

**FWP and possible subtask under FWP:**

Crystallography of Microstructures (sub-task: New Al-Si-Ge Alloys for Automobile Applications)

**FWP Number:** KC11

**Program Scope:** Investigate the fundamental features that underlie the evolution of microstructures in solids by applying crystallographic techniques to the analysis of topology and defects in crystalline materials. Understand and ultimately gain control of the structure, distribution and shape of defects such as inclusions, grain boundaries, domain walls and dislocations by establishing the basic relationship between crystallographic variables and structural observables. Such relationships are put to use both analytically, to examine the structure of defects, and synthetically, to produce new and unique microstructures with defect configurations reflecting composite symmetries. Because of the scale and nature of such microstructures, electron microscopy is an integral part of these investigations, as an analytical tool as well as a subject of technique development.

**Major Program Achievements (over duration of support):**

The failure of nanosized Pb inclusions in Al to reach their equilibrium shape was found to be due to a fundamental kinetic limitation characteristic of faceted nanoparticles. The Pb/Al interface was shown for the first time to undergo a roughening transition at about 550°C. Quantitative in-situ observations by TEM established the degree of anisotropy and the magnitude of the step energy in the interface.

Nanoscale lead-tin alloy particles with sizes from 2 to 20 nm, embedded in Al, were found to have size-dependent solubilities. Fine-probe EDX analysis on the two-phase inclusions showed that both phases were supersaturated, and their concentrations were considerably higher than allowed by the phase diagram. Inclusions less than 10 nm in size nearly always displayed a single phase fcc structure with tin concentrations as high as 50 at. %.

Epitaxial fcc, bcc and hcp metal and alloy films grown by on Si and Ge surfaces at different deposition temperatures were characterized by TEM and diffraction. The different epitaxial relationships could be understood and utilized to generate Potts model microstructures of different orders.

A detailed TEM analysis was able to explain the unique combination of ultra-rapid aging response, high peak hardness and extended aging microstructural stability of quaternary Al-Cu-Si-Ge alloys. Si-Ge particles act as nucleation sites for  $\theta'$  precipitates, resulting in a peak aged microstructure with a dense distribution of  $\theta'$  precipitates attached to Si-Ge.

**Program Impact:**

This work has led to an improved understanding of the key role played by interface structure in the evolution of microstructures. In particular, the role of crystallographic alignment and confinement in a solid matrix on the behavior of nanoscale particles has been elucidated and utilized in thin film growth and precipitation reactions.

**Interactions:**

CEA Grenoble, Dept. Recherche Fondamentale sur la Matière Condensée (F. Lançon)  
University of Copenhagen, Oersted Lab (E. Johnson)  
University of Belgrade, Dept. of Materials Science (V. Radmilovic)

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

22 Invited talks since 2001

**Personnel Commitments for FY2002 to Nearest +/-10%:**

U. Dahmen (group leader) 40%  
V. Radmilovic (staff scientist) 50%  
T. Radetic (post-doc) 100%  
F. Lançon (visiting scientist from CEA Grenoble) 20%

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$370,000

**FY01 BA** \$355,000

**FY02 BA** \$358,000

**FWP and possible subtask under FWP:** Metals Program: Engineering the Limits of Strength  
**FWP Number:** KC12

**Program Scope:** Prediction, measurement and control of the limits of strength for structural materials. This program seeks to develop and apply novel experimental and theoretical techniques in order to predict, to understand the origins of, and to engineer the extreme strengths of structural materials. Materials studied include BCC metals and alloys (including ultra high strength steels), FCC metals, and diamond cubic and zincblende semiconductors (materials that are increasingly being exploited for their structural properties in Micro ElectroMechanical Systems or MEMS).

**Major Program Achievements (over duration of support):** Ideal Tensile and Shear Strength of BCC metals and alloys: We have investigated theoretically the ideal shear and tensile strengths of a number of BCC metals and alloys. Computed results for the ideal shear and strengths of W and Mo are in excellent agreement with values deduced from nanoindentation experiments. Studies of the ideal strength of Fe indicate the important role that spin plays in its strength.

TEM *in situ* Nanoindentation: In collaboration with NCEM, we have developed the next generation TEM *in situ* nanoindentation apparatus. We have used this device to study the properties of Al, grain boundaries in Al, diamond-like carbon, and Si. We have observed directly dislocation loop punching (driven by the indenter tip), and a surprising level of dislocation activity in Si.

Dislocation Core Structures: We have developed methods for computing the relative energies and the structures of dislocation cores in diamond cubic and zincblende semiconductors and have applied these techniques to predict the stress state dependence of dislocation cores in diamond, Si and more recently GaAs. We have compared, directly and quantitatively, computed core structures with the results of High Resolution Electron Microscopy experiments. Fatigue of MEMS: We have designed a novel MEMS based testing configuration to explore the fatigue of Si within MEMS structures. These experiments demonstrate conclusively that MEMS devices do fatigue.

**Program impact:** We developed a deep understanding of the upper limit of strength and proved that this limit is accessible to experimental measurements: This constitutes a genuine prediction of a nontrivial mechanical property. These studies led to the identification of the crystallographic factors limiting ductility, and can therefore guide efforts to develop hard coatings and ultra-high strength steels (for example). We also developed a deep understanding of the factors impacting computation and experimental measurement of dislocation core structures. The quantitative comparison between experimentally determined and predicted structures serves to guide development of models for the mechanical properties of the studied material, and also allows detailed analysis of imaging artifacts thus enabling the development of improved high resolution electron microscopy techniques. Finally, the TEM *in situ* nanoindenter provides access to experimental information not previously accessible. This instrument will be involved in a broad spectrum of materials investigations and will advance substantially our understanding of the mechanical properties of many materials.

**Interactions:**

National Center for Electron Microscopy (NCEM), LBNL; Advanced Light Source, LBNL; Sandia National Laboratories, Albuquerque; Frederick Seitz Materials Research Laboratory, University of Illinois; Inha University, Korea; Hanyang University, Korea; National Energy Research Scientific Computing Center, LBNL.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Fellow, The Metallurgical Society (TMS), 2001 (Morris); Lee Hsun Memorial Lecturer, Inst. Metals Research, Chinese Academy Science, 2002 (Morris); Key speaker at Extended Defects in Semiconductors 2002, Bologna, Italy (Chrzan); Invited speaker at Gordon Research Conference on Point and Line Defects in Semiconductors, 2002 (Chrzan); More invited talks, awards and honors too numerous to list here.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

**Chrzan** (PI) 20%; Morris (PI) 20%; Ritchie (PI) 10%; 2 Visiting Scholars (no cost to DOE); 1 Post-Doc (100%); 8 students supported (on average) for 70% of their time; 2 additional students on fellowship working at no cost to DOE.

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$652,000

**FY01 BA** \$652,000

**FY02 BA** \$660,000

**Laboratory Name:** Lawrence Berkeley  
National Laboratory  
**B&R Code:** KC020103

**FWP and possible subtask under FWP:** Electronic Materials Program

**FWP Number:** KC12

**Program Scope:**

The program goal is to advance the fundamental understanding of the complex materials science of semiconductor systems and devices. The research focuses on the relationships between synthesis and processing conditions and the structure, properties, and stability of semiconductor materials systems. Progress in this area is essential for the performance and reliability of future high efficiency light sources, visual displays, photovoltaic energy conversion devices, security systems, communication technology, and of a large variety of sensors and power control systems for energy generation, conservation, distribution and use.

**Major Program Achievements (over duration of support):**

Developed new and predictive theory (band anticrossing model) to explain properties of “highly mismatched” semiconductor alloys (HMAs) such as  $\text{GaN}_x\text{As}_{1-x}$ , discovered new II-VI HMAs, and contributed significantly to the understanding of InN as a narrow gap semiconductor; many of these materials show promise as components of high efficiency solar cells and other opto-electronic devices. Performed fundamental studies of extended defects, compositional fluctuations, and the resulting strain distributions; results were used to understand the light emission mechanism in GaN and InGaN materials used for solid state lighting. Pioneered scientific applications of isotopically controlled semiconductors; performed definitive diffusion studies in Group IV and III-V semiconductors using stable isotope superlattices. Developed fundamental understanding of the relationship between native defects and the achievable limits for semiconductor doping. Designed a new, patented lateral overgrowth process for nitrides. Determined the atomistic core structure of dislocations in group III nitride semiconductor thin films and heterostructures.

**Program Impact:** Over the course of many years of sustained BES funding, the Electronic Materials Program has discovered new classes of semiconducting materials (e.g., II-VI HMAs) and has contributed significantly to the synthesis and fundamental understanding of a large number of Group IV and III-V semiconductors.

**Interactions:**

Internal—National Center for Electron Microscopy, Advanced Light Source.

External—Stanford Synchrotron Radiation Laboratory, Hewlett-Packard, Agilent, MPI Stuttgart, Xerox, NREL, Cornell Univ., Purdue Univ., Univ. of Notre Dame, Harvard Univ., Münster Univ., Germany

**Recognitions, Honors and Awards (at least in some part attributable to support under this program):**

J. W. Ager III – co-editor, Topical Issue of *Semiconductor Science and Technology*, “Group III-N-V Alloys,” 2002.

E. E. Haller – Recipient James C. McGroddy Prize for New Materials of the American Physical Society, 1999; Chair, 20th Intl. Conf. on Defects in Semiconductors (20th ICDS), Berkeley, CA 1999; Recipient Max-Planck Research Award, 1994; Research Professor, Miller Foundation for Basic Research in Science, 1990 and 2001; Fellow, American Physical Society, 1986; A. von Humboldt US Senior Scientist Award, 1986.

Z. Liliental-Weber – Chair, IEEE Semiconducting and Insulating Materials Conference (SIMC-X), Berkeley, CA 1998.

W. Walukiewicz – co-editor, Topical Issue of *Semiconductor Science and Technology*, “Group III-N-V Alloys,” 2002, NTT distinguished Professorship 1990.

E. R. Weber – Fellow, American Physical Society (APS), 2001; Humboldt Senior US Scientist Award, 1994.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

E. E. Haller (20%), J. W. Ager III (20%), E. D. Bourret-Courchesne (70%), O. D. Dubon, Jr. (10%), Z. Liliental-Weber (50%), W. Walukiewicz (80%), J. Washburn (25%), E. R. Weber (10%), K. M. Yu (50%).

**Authorized Budget (BA) for FY00, FY01, FY2002:**

**FY00 BA** \$1,156,000

**FY01 BA** \$1,253,000

**FY02 BA** \$1,322,000

**Laboratory Name:** Lawrence Berkeley  
National Laboratory  
**B&R Code:** KC0201030

**FWP and possible subtask under FWP:** Ceramics Program  
**FWP Number:** KC12

**Program Scope:**

A multidisciplinary investigation of interface composition, structure/bonding and macroscopic properties in ceramics to provide new information on atomic structure and relations to the properties of ceramics and ceramic interfacial structures. Specifically, to examine ceramic grain boundaries and dissimilar interfaces in order to evaluate interface-dependent properties, including mechanical and thermo-chemical stability and kinetic behavior.

**Major Program Achievements (over duration of support):**

Developed *in situ* toughened silicon carbide (ABC-SiC) with combinations of very high fracture toughness and excellent creep, wear and fatigue strength up to 1300-1400°C. Characterized the morphology, crystal structure and chemistry of nanoscale intergranular films, and related microstructural evolution at elevated temperatures. Determined the worst-case cracking thresholds and intrinsic toughness of self-reinforced alumina and SiC ceramics. Developed statistical models for the crack initiation toughness, crack-path directionality and crack kinking in functionally-graded materials. Developed crack-free joining technique for alumina and silicon nitride using functionally-graded bonding layers. Evaluated the interface chemistry and its relation to strength, fracture and fatigue resistance of alumina bonded with aluminum and Cu/Nb transient liquid-phase interlayers. Also evaluated the chemistry at alumina/alloy interfaces during high temperature oxidation and its relation to interfacial void formation, oxide growth processes and scale adherence. Demonstrated the presence of multi-layered interface structures from impurity segregation, which have marked effects on bonding strength and widespread implications on multi-component interfacial adsorption. Developed new models for ridge-limited high-temperature liquid spreading. Analyzed the wetting behavior of PbO-Nb<sub>2</sub>O<sub>3</sub> and PbO-TiO<sub>2</sub> glasses on dense PbZrTiO<sub>3</sub> (PZT). Established the pressure dependence of surface, interface, and ceramic grain-boundary energies for liquid metals on ceramics with oxygen partial pressure.

**Program Impact:** Development of a series of silicon carbide ceramics with unparalleled combinations of low-temperature strength/toughness and outstanding high-temperature creep/fatigue properties; radical re-evaluation of the classic Young-Dupre Equation for the contact angle/wetting behavior of liquid metals on ceramic surfaces.

**Interactions:**

Internal—National Center for Electron Microscopy, Advanced Light Source, MSD Metals Program.

External—Oak Ridge National Laboratory; Lawrence Livermore National Laboratory; Sandia National Laboratory; Argonne National Laboratory; Los Alamos National Laboratory; Idaho Engineering National Laboratory; National Institute of Standards and Technology; MIT; Carnegie Mellon University; Crystal Systems Inc.; Osram Sylvania; General Electric; Eindhoven University of Technology; Institute for Advanced Materials, Petten; Max-Planck Institute, Stuttgart, Germany.

**Recognitions, Honors and Awards (at least in some part attributable to support under this program):**

R.M. Cannon – *Humboldt Research Award* for senior US scientist.

L.C. DeJonghe – *Engineering Alumnus of the Year*, Materials Science, University of Delaware.

P.Y. Hou – Chair, Gordon Conference on High Temperature Corrosion

R.O. Ritchie – elected to *National Academy of Engineering* and the *Royal Academy of Engineering*, London.

A.P. Tomsia — *Humboldt Research Award* and *IUMRS Somiya Award* for International Collaboration.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

R. O. Ritchie (15%), R. M. Cannon (70%), L. C. DeJonghe (10%), A. M. Glaeser (10%), P. Y. Hou (60%), J. J. Kruzic (100%), E. Saiz (40%), A. P. Tomsia (40%), X.-F. Zhang (100%)

**Authorized Budget (BA) for FY00, FY01, FY2002:**

**FY00 BA** \$1,561,000

**FY01 BA** \$1,469,000

**FY02 BA** \$1,368,000

**Laboratory Name:** Lawrence Berkeley National Laboratory  
**B&R Code:** KC020202, KC020105, KC020203

**FWP and possible subtask under FWP:**  
Superconductivity

**FWP Number:** KC22, KC21, KC23

**Program Scope:** Development of low-and high-transition temperature ( $T_c$ ) Superconducting QUantum Interference Devices (SQUIDs) and their application to a broad range of phenomena. Low- $T_c$  SQUIDs: nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) in ultralow magnetic fields at frequencies as low as 100 Hz; multiplexers for readout of bolometers for far infrared and submillimeter astronomy; novel microstrip resonator configuration for axion detectors and detection of quantum coherence; measurement of magnetic fields from the heart to diagnose heart disease. High- $T_c$  SQUIDs: development of novel gradiometers for magnetocardiography in an unshielded environment; detection of magnetic nanoparticles bound to bacteria as a new biosensor; nondestructive evaluation of fatigue in steel after fatigue cycling.

**Major Program Achievements:** SQUID detection of NMR and MRI at ultralow frequencies enables both very narrow linewidths (1 Hz) and high spatial resolution (1 mm) even in grossly inhomogeneous magnetic fields. Splittings due to scalar (J) couplings of 10 Hz in a field of 5 microtesla demonstrated. First demonstration of high-sensitivity dc SQUID fabricated from the new superconductor  $MgB_2$ . Eight-channel SQUID multiplexer replaces 8 SQUIDs and ancillary equipment with a single SQUID. Noise temperature within a factor of two of the quantum limit at 0.5 GHz achieved with microstrip SQUID amplifier. Biosensor based on high- $T_c$  SQUID detects pathogens with sensitivity and specificity that compare favorably with commonly used techniques.

**Program Impact:** SQUID-based NMR and MRI under active consideration for commercial development; SQUID multiplexer being developed to read out bolometer arrays on ground-based telescope; SQUID microstrip amplifier is being used in circuits to demonstrate quantum coherence.

**Interactions:** Internal: M.D. Alper (MSD, LBNL); E.L. Hahn (Physics, UCB); A.T. Lee (Physics, UCB); J.W. Morris (Materials Sciences, UCB and MSD, LBNL); A. Pines (Chemistry, UCB and MSD, LBNL); P.L. Richards (Physics, UCB); H. Spieler (Physics, LBNL); V. Vreeland (MSD, LBNL). External: A.A. Bakharev (CardioMag Imaging, Inc., Schenectady, NY); G.W. Crabtree (ANL); P. Delsing (Chalmers University, Sweden); M. DiIorio (MagneSensors, Inc., San Diego), A.C. Gossard (Materials Dept., UCSB); D. Kinion (LLNL); M. Mueck (University of Gießen, Germany); P. Thomson (Cardiology, Alta Bates Hospital, Berkeley).

**Recognitions, Honors and Awards:** J. Clarke – IEEE Award for Continuing and Significant Contributions in the Field of Applied Superconductivity (2002); J. Clarke and A. Pines – named as Research Leader in General Technology in Scientific American 50 (2002); SQUID Multiplexer, highlighted in Physics News (2001); J. Clarke – Chair-Elect, Chair, Past Chair of DCMP, APS (2000-2002); Chair, APS March Meeting (Seattle, 2001); Program Committee and/or International Advisory Committee for: International Superconductive Electronics Conferences, Osaka, Japan (2001) and Sydney, Australia (2003); Physics and Applications of SQUIDs, Stenungsbaden, Sweden (2001); International Symposium on Superconductivity, Tokyo, Japan (2000), Kobe, Japan (2001), Yokohama, Japan (2002); Editorial Boards of Journal of Low Temperature Physics and Superconductor Science and Technology. 59 invited talks (FY00-02).

**Personnel Commitments for FY2002:**

J. Clarke (program leader) 25%; gsr's (62.5%): J. Chen, H. Grossman, N. Kelso (zero time charged to project), S-K. Lee, R. McDermott, W. Myers, R. Therrien, D. Kinion (postdoc) 80% (zero time charged to project).

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$515,000

**FY01 BA** \$507,000

**FY02** \$376,000

**Laboratory Name:** Lawrence Berkeley National Laboratory  
**B&R Code:** KC020301 in 2003 B&R KC020601

**FWP and possible subtask under FWP:** Characterization of Functional Nanomachines

**FWP Number:** MSD-NAN002-02

**Program Scope:**

Development and application of controllable, operational nanomachines and nanomotors from molecular building blocks. Determination of the mechanisms of chemical-to-mechanical energy transfer in naturally occurring molecular bio-motors and artificial bio-motor assemblies. Chemical synthesis of new molecules having tailored geometry, electro-activity, and surface reactivity for use as nano-machine components. Local probe study of functional molecules adsorbed to surfaces and actuated using optical and electronic stimulus. Use of combined MEMS technology and fullerene growth techniques to create electro-mechanically actuated molecular motors from carbon nanotubes. Theoretical prediction and explanation of nano-motor behavior through *ab initio* electronic structure calculations.

**Major Program Achievements (over duration of support):**

Fabrication of voltage-operated nanotube-based mechanical actuator. Successful synthesis of functionalized azobenzene molecules in high purity crystalline form for UHV sublimation. Initial tests performed to evaporate azobenzene derivatives onto clean Si surface. LDA calculations performed to predict excited state induced conformational changes in adsorbed azobenzene molecules. Optical tweezer investigations performed into the mechanism by which the portal motor of bacteriophage phi29 couples ATP hydrolysis to generate force during the packaging of viral DNA into the capsid.

**Program impact:**

Successful beginning of integrated synthesis, experiment, and theoretical effort to explore molecular machine components. First fabrication of voltage-operated nanotube-based mechanical actuator capable of operation at high and low temperature and in UHV environment

**Interactions:**

Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory  
External: IBM Almaden, Yale, University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, SUNY Stony Brook, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

None yet.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

No personnel money has been spent yet, but time commitments have been made, as follows: M. F. **Crommie** (PI) 35%, C. Bustamante (co-PI) 20%, J. Frechet (co-PI) 15%, A. Zettl (co-PI) 20%, S. Louie (co-PI) 15%, M. L. Cohen (co-PI) 15%, Y. Chemla (postdoc) 100%, K. Nagaoka (postdoc) 50%, M. Comstock (grad. student) 50%, G. Begtrup (grad. student) 100%

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$0

**FY01 BA** \$0

**FY02 BA** \$800,000

**Laboratory Name:** Lawrence Berkeley National Laboratory

**B&R Code:** KC020202

**FWP and possible subtask under FWP:** Manybody Processes and Quantum Size Effects in Semiconductor Nanostructures and Correlated Electron Systems

**FWP Number:** KC22

**Program Scope:** Explore quantum size effects, many-body interactions and new thermodynamics in nanostructures and low dimensionality materials. A particular emphasis is put on Coulomb Correlation since in low dimension systems quasi-particles have fewer degrees of freedom to avoid each other and Coulomb mediated many-body interactions become dominant.

**Major Program Achievements:** Because of space limitation only the last 4 years are reviewed, in that period the program produced 30 publications in peer reviewed journals, including 3 in Nature, 11 in Phys. Rev. Letters and 10 in Phys. Rev. B. Solution of the four-decades old problem of the polariton transmission in the slab geometry. First unambiguous observation of 4-particle correlations effects in a micro-cavity. First observation and theory of 4-particle correlations in semiconductors using the tunable magnetic fields enhancement of exciton-exciton interaction. First observation of high order (at least 6-point functions) Coulomb correlations in the optical response of semiconductor quantum wells at extremely low density on time-scales short compared to the time between quasi-particle collisions and demonstration of breakdown of the Random Phase Approximation. First experimental and theoretical investigations of intra-Landau-level and inter-Landau-Level quantum coherence of electron-hole pairs in the presence of a two-dimensional electron gas in the Quantum Hall Effect regime. First observation of condensation of highly degenerate exciton gas in in-plane traps of coupled quantum well structure. First observation of a new macroscopically (~1mm) ordered state in degenerate exciton gas. First investigation of the renormalization of the spin-wave band structure through generation of non-equilibrium populations of antiferromagnetic spin-waves in the transition metal oxide, Cr<sub>2</sub>O<sub>3</sub>. First observation of even-parity excitations in the strongly correlated charge-transfer insulator, Sr<sub>2</sub>CuO<sub>2</sub>Cl<sub>2</sub>, by optical third harmonic generation spectroscopy. First study of the optical conductivity of MgB<sub>2</sub> covering the range of its superconducting energy gap by Terahertz time-domain spectroscopy.

**Program Impact:** Understanding many particle systems in one of the outstanding issues of modern physics. This problem is most pronounced in condensed matter physics because here “quasi-particles” are complex objects with an internal structure, strongly interacting among themselves in the background of a “vacuum” itself dynamical and structured. Quantum size effects appear when the dimensions of a system become comparable or smaller than the characteristic lengths that govern the quantum mechanics of the process under investigation. In particular a number of approximations (as fundamental as the Random Phase Approximation) or theoretical approaches (such as Boltzmann Kinetics) can cease to be valid in nanoscale systems, especially on very short time scales. This opens the way for a wealth of unprecedented investigations, and provides new opportunities to test our understanding of fundamental physical processes in regimes previously inaccessible. Furthermore, properties of nanometer materials can be engineered at the atomic level to optimize their functionality for specific applications. These new and atomically designed artificial materials have the potential to revolutionize materials sciences, and to produce devices with highly improved performances.

**Interactions:**

Prof. A. Gossard, University of California at Santa Barbara. Prof. J. Orenstein and Prof. P. Alivisatos University of California at Berkeley. H. M. Christen and D. H. Lowndes, Solid State Division, Oak-Ridge National Laboratory, Prof. I. Perakis, University of Crete, Greece. Prof. W. Schäfer, Jülich Forschungszentrum, Germany. Prof. J. Tignon, Ecole Normale Supérieure de Paris, France

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Member of the National Academy of Sciences

Fellow: Physical Society of America, IEEE-Laser and Electro-Optic Society, Optical Society of America

1988 R.W. Wood prize of the Optical Society of America, 1995 Quantum Electronics Award of the IEEE Laser and Electro-Optics Society, 1995 Humboldt Research Prize, 1998 Gordon Conferences A. M. Cruikshank Lecturer

**Personnel Commitments for FY2002:** Daniel Chemla (Group Leader) 40% (0% funding), Leonid Butov (Sci. Staff) 100%, R. Kaindl (Post Doc) 100%, C-W Lai (Graduate Student) 100%, M. Carnahan (Graduate Student) 100%, B. Schmid (Graduate Student) 100%, A. Minstev (Visiting Graduate Student from Russia) 25%

**Authorized Budget (BA):**

**FY00 BA** \$429,000

**FY01 BA** \$427,000

**FY02 BA** \$513,000

**FWP and possible subtask under FWP:**

Surface, Interface & Nanostructure Studies Using Synchrotron Radiation in Combination with Other Methods  
**FWP Number: KC22**

**Program Scope:**

This project utilizes advanced spectroscopic and structural techniques based upon third-generation synchrotron radiation, together with complementary methods (e.g. LEED, STM, SMOKE, TEM), to study atomic structures and electronic and magnetic properties of surfaces, interfaces, nanostructures, and bulk materials. Problems studied include: magnetic multilayers, interface effects on giant magnetoresistance and exchange biasing, short-range versus long-range magnetic order in the colossal magnetoresistive (CMR) oxides and diluted magnetic semiconductors, metal-oxide-metal magnetic tunnel junctions, the electronic structure of fullerene cage materials, and kinetics and structure in surface reactions such as oxidation of metals and semiconductors. Techniques utilized include angle-resolved photoelectron spectroscopy, diffraction, and holography; x-ray absorption; x-ray emission; and x-ray elastic and inelastic scattering. Spectroscopies excited by soft x-ray standing waves and x-ray fluorescence holography are under development. Experiments at the ALS use several unique experimental systems, including a photoelectron spectrometer/diffractometer located on an elliptically polarized undulator. This program also has a strong theoretical component directed toward interpreting spectroscopy, diffraction and holography.

**Major Program Achievements (over duration of support):**

During the past two years, we have developed a new standing wave method for spectroscopically studying buried interfaces in nanostructures, observed for the first time a high-temperature electronic phase transition in the CMR oxides, and significantly improved the instrumentation and detectors available for both spectroscopic and x-ray holographic studies at the Advanced Light Source.

**Program impact:**

Major impacts include: developing a new and generally useful standing-wave method for studying buried interfaces via the soft x-ray spectroscopies (photoemission, x-ray emission, x-ray absorption); establishing a better understanding of the high-temperature electronic structure in the CMR materials, with implications also for phase separation in the high TC materials; and developing ultrahigh speed detectors for synchrotron radiation research to enable the next generation of such studies.

**Interactions:**

Internal: LBNL (M. Van Hove, J. Kortright, M. Salmeron, Z. Hussain); External: University of California-Davis (W. Pickett, R. Singh, K. Liu); LLNL (A. Szoke, H. Chapman); ANL (J. Mitchell); IBM Almaden (S.S.P. Parkin); Univ. of the Basque Country (F. Garcia de Abajo); Ben-Gurion Univ. (M. Polak); Univ. of Tokyo (T. Ohta); Beijing Synchrotron Radiation Laboratory (K. Ibrahim); Correlated Electron Research Center, Japan (Y. Tokura and Y. Tomioka); Hong Kong Univ. of Science and Technology (S.-H. Yang)

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

32 invited talks at national or international conferences or summer schools over 1999-2002  
Special issue of the Journal of Electron Spectroscopy and Related Phenomena honoring C.S. Fadley  
Paper on standing wave spectroscopy chosen for special recognition by the Institute of Physics (IOP Select--  
<http://www.iop.org/Select/G/3/100/>).

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

C.S. Fadley (50%), M. West (50%), M. Press (25%), N. Mannella (50%)

**Authorized Budget (BA) for FY00, FY01, FY02:**

FY00 BA \$430,000

FY01 BA \$433,000

FY02 BA \$400,000

**FWP and possible subtask under FWP:**

Resonant Soft X-Ray Studies of Nanostructured Magnetic Materials

**FWP Number:** KC22

**Program Scope:**

Develop instrumentation and techniques to utilize unique attributes of core-resonant soft x-ray magneto-optical effects, and apply these techniques to gain fundamental insight in current and emerging magnetic materials, especially heterogeneous and nanostructured materials. Techniques include intensity and polarization-resolved *spectroscopies* that sense laterally-averaged, element- and depth-resolved magnetic and chemical properties, as well as *scattering* and *microscopy* to probe lateral heterogeneity in these properties at length scales down to 1 nanometer. Photon-based techniques are emphasized because of their penetrating power and compatibility applied fields.

**Major Program Achievements (over duration of support):**

Developed unique endstation for soft x-ray magneto-optical studies in fields up to 1.5 Tesla and with temperature. Developed standing-wave enhanced magnetic circular dichroism technique for the study of magnetic and chemical variations across buried interfaces. Developed resonant small-angle scattering techniques to study magnetic and chemical heterogeneity and applied them in a variety of granular alloy, multilayer, and nanoparticle systems having both in-plane and perpendicular anisotropy. Extended incoherent scattering techniques into the coherent scattering (magnetic speckle) regime. Developed polarization-resolved x-ray magneto-optical Kerr effect measurements and applied them to resolve depth-dependent magnetization changes in exchange-spring and exchange-bias structures. Developed techniques for magnetic imaging using existing scanning transmission x-ray microscope. Extended core-resonant scattering techniques for first studies of heterogeneous polymer systems at the carbon K edge.

**Program impact:**

This program has demonstrated that well-known techniques such as scattering and diffraction from the hard x-ray spectral range, and magneto-optical spectroscopies and microscopies from the near-visible spectral range, can be beneficially extended into the soft x-ray spectral range, where they gain added value from application at relevant core levels. In addition to experimental capabilities, rigorous analytical techniques have attracted collaborators from industry, national labs, and universities to form the nucleus of a growing program at the ALS to further their development and extend the application of these techniques to a broader range of systems of both fundamental and technological interest involving magnetic heterogeneity at the nanoscale.

**Interactions:**

IBM Almaden Research Center (E.E. Fullerton); LBNL (C. F. Fadley, Center for X-Ray Optics, ALS); Argonne National Lab (S.D. Bader); Motorola (J. M. Slaughter); U. Oregon (S. D. Kevan); U. Washington (L. Sorenson); U. Penn (N. Samarth); U. Colorado (D. Desseau).

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

10 invited talks since 2000.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

J. B. Kortright (PI) 100%

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$215,000

**FY01 BA** \$230,000

**FY02 BA** \$214,000

**Laboratory Name:** Lawrence Berkeley National Laboratory

**B&R Code:** KC020202

**FWP and possible subtask under FWP:**

Spin, lattice and electronic properties of novel complex materials.

**FWP Number:** none

**Program Scope:**

The PI has just recently become a member of this DOE program. The following points summarize the scope of her research: 1) Study of elementary excitation and investigation of concomitant role of spin, charge and orbital degrees of freedom in strongly correlated systems, non-magnetic and magnetic nanostructures; study of reduced or confined dimensionality in mesoscopic systems, nanostructures, nanosphere and nanorods. The approach is to combine angle and spin resolved photoemission spectroscopy with circularly polarized light.

2) Study of the nanoscale spatial and temporal fluctuations in strongly correlated materials by using scattering of spatially coherent soft X-ray (soft X-ray Speckle).

3) Development of a new spin polarized detector system (at the Advanced Light Source) based on a novel concept of time of flight energy analyzer, with expected unprecedented high energy and momentum resolution and high collection efficiency.

4) The PI is also actively involved in the project for the development of a new experimental facility ("New meV resolution Beamline") at the Advanced Light Source. The new facility will combine together Angle and Spin Resolved Photoemission Spectroscopy with Resonant Inelastic X-ray Scattering.

**Major Program Achievements (over duration of support):**

As a new member of this program the projects carried out in the PI's lab are only in their initial stages. Following are the details for each project: 1) Preparation of single wall carbon nanotubes for photoemission spectroscopy to investigate the reported Luttinger liquid behavior. 2) Experimental setup and first data recording on Soft X-ray scattering experiment on striped LSCO superconductor. 3) By combining expertise in different field (Chemical Material Division, Material Science Division and Electron Center for Electron Microscopy at the LBL in Berkeley) the project of the new spin resolved photoemission analyzer has actively started (experimental testing of single component and design).

**Program impact:**

The impact of the following research activity will contribute to our understanding of the role of various degrees of freedom in complex materials and the role of nanometer scale dynamical fluctuations. These, combined together with study of nanostructures materials will help in our understanding of how to engineer new materials with desired properties.

On the other hand the development of a new Spin detector and *meV* Beamline facility will enable the investigation of a wider range of materials improving our current understanding of condensed matter physics. This will also allow addressing new regimes never investigated until now, and will be fundamental to the engineering of new materials with desired properties.

**Interactions:**

Internal — Advanced Light Source (ALS); Chemical Science Division; National Center for Electron Microscopy; Material Science Division; Department of Physics and Chemistry, University of California Berkeley.

External— Stanford University; University of Tokyo, Japan; Electrotechnical Laboratory (ETL), Tsukuba, Japan; Università Cattolica Brescia, Italy; Università di Roma I, Italy; Sincrotrone Trieste, Elettra, Italy.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

The PI has joined this DOE program only few months ago. However part of her new work is a continuation on a recent in the field of high temperature superconductors which not only has greatly influenced the direction of research in the field but has received a big amount of media coverage and press releases in various countries (Italy, Germany, Japan, USA). During this last year the PI has been co-organizer of a workshop at the Advance Light Source, aimed to the development of the new facility (see point 3), and has been invited more than 15 times to conferences and other institutions to present her new work.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

Alessandra Lanzara (PI) 100%; Gey-Hong Gweon (Post-doc) 100%, Jeff Graff (Visiting researcher) 100%

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA \$ 0**

**FY01 BA \$ 0**

**FY02 BA \$ 0**

**FWP and possible subtask under FWP:**

Time-resolved optical spectroscopy of correlated electron systems

**FWP Number:** KC22

**Program Scope:**

Development of advanced techniques of time-resolved optical spectroscopy and application to systems of correlated electrons. High-precision time-domain spectroscopy exploring the linear and nonlinear response of superconductors in the terahertz frequency domain. Heterodyne detection of transient grating allowing direct real-space observation of the propagation of quasiparticles in correlated electron metals.

**Major Program Achievements (over duration of support):**

Pioneered research in terahertz optical conductivity of the vortex state of high-T<sub>c</sub> superconductors. First observation of the optical Hall conductivity of both quasiparticles and vortices. Precision measurements of the dissipation due to vortex motion at high frequencies.

Direct measurement of the rate of phase fluctuations of the superconducting order parameter in a high-T<sub>c</sub> superconductor. Demonstration that phase transition from superconducting to normal state is driven by phase fluctuations. Proof of absence of superconducting fluctuations in the pseudogap regime.

First measurement of the quasiparticle scattering rate in the high-T<sub>c</sub> superconductor BSCCO by optical conductivity measurements. Identification and theoretical explanation of a component of the optical conductivity originating from extreme heterogeneity of the local superfluid density.

First direct observation of quasiparticle propagation in a high-T<sub>c</sub> superconductor, using heterodyne transient grating spectroscopy. Time-resolved detection of quasiparticle motion lead to direct measurement of the quasiparticle diffusivity tensor, inelastic, and elastic scattering rates in high-quality YBCO untwinned single crystals.

**Program impact:**

Recognized internationally as leading group using advanced laser-based techniques to discover effects and obtain data not available using conventional spectroscopic methods.

**Interactions:**

University of Illinois (Prof. J. Eckstein)

Los Alamos (Dr. A. Ramirez)

University of British Columbia (Profs. W.N. Hardy and D.A. Bonn)

Stanford University (Prof. M. Beasley)

**Recognitions, Honors and Awards**

Chair, Gordon Conference on Correlated Electron System (2002-present)

Vice-chair, Gordon Conference on Correlated Electron Systems (2002)

Chosen by editors of Science to write review of advances in the physics of high-T<sub>c</sub> superconductors

International and national invited talks, including APS March Meeting, Aspen Center for Physics, Institute for Theoretical Physics (Santa Barbara), International Center of Physics (Trieste), Gordon Conference on Superconductivity (Oxford, UK), and Symposium on SPC Coupled Materials (Tokyo).

**Personnel Commitments for FY2002 to Nearest +/- 10%: J. Orenstein (group leader) 30%**

Nuh Gedik (grad student) 100%

Matthew Langer (grad student) 100%

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$ 118,000

**FY01 BA** \$169,000

**FY02 BA** \$193,000

**FWP and possible subtask under FWP:** Spectroscopy and Microscopy, subtask on Surface Magneto-Optic Kerr Effect

**FWP Number:** KC22

**Program Scope:**

This research program aims to fabricate, characterize, and explore new properties of magnetic nanostructures synthesized by the state-of-the-art of the Molecular Beam Epitaxy (MBE) technique. Spectroscopy on the valence electrons and microscopy on the core electrons were measured at the Advanced Light Source (ALS) to explore the electron confinement (quantum well states) and the element-specific magnetic domain properties in magnetic nanostructures. In addition, Surface Magneto-Optic Kerr Effect (SMOKE) was applied to measure the magnetic hysteresis loops to obtain the macroscopic magnetic properties.

**Major Program Achievements (over duration of support):**

Achievements were made in the following three different areas.

**Spectroscopy Study of the Quantum Well (QW) States:** Scanning photoemission experiments are performed across wedged Cu/Co/Cu(100). We show that the QW states in the Cu thin films can be described by the envelope function of the Bloch wave, and the oscillatory magnetic coupling is determined by the QW states at the belly and neck of the Fermi surface.

**Microscopy Study of the Ni/Fe/Co/Cu(100):** Using PEEM to do element-specific magnetic domain imaging at the ALS, we explored the Ni, Fe, and Co domain relations in Ni/Fe/Co/Cu(100). We found that the fcc Fe produces an oscillatory interlayer coupling between the Ni and Co films, and this interlayer coupling results in an oscillations of the Ni film Curie temperature.

**SMOKE Study of Stepped Thin Films:** SMOKE technique was used to investigate magnetic thin films grown on vicinal surfaces. The atomic steps break the rotation symmetry to generate the magnetic anisotropy. Using curved substrate, we are able to explore the role of the lattice symmetry in the magnetic anisotropy.

**Program Impact:**

This program provides a fundamental understanding on a series of newly discovered phenomena in magnetic nanostructures. In addition, microscopic knowledge from this study provides useful guidance for future synthesis of magnetic nanostructures with new properties.

**Interactions:**

Advanced Light Source

National Center of Electron Microscopy

Materials Science Division and Supercomputer Center

**Recognitions, Honors and Awards (at least in some part attributable to support under this program):**

Five invited talks were given at domestic and international conferences.

1. "Quantum well states in magnetic nanostructures", APS March Meeting (Minneapolis), March. 2000.
2. "Lateral modulation of magnetic thin films using curved substrate", International Symposium on Physical Properties of Structural Thin Films, Freie Univ., Berlin, Germany, April 12-13, 2000.
3. "Quantum well states in magnetic nanostructures" 16th International Colloquium on Magnetic Films and Surfaces (Brazil), August 14-18, 2000.
4. "Quantum well states and interlayer coupling in magnetic nanostructures", The 13th International Conference on Vacuum Ultraviolet Radiation Physics (Trieste, Italy), July 22-27, 2001.
5. "Electron confinement in metallic ultrathin films", 49th American Vacuum Society Conference (Denver), Nov., 2002.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

Z. Q. Qiu PI (25%), W. L. Ling (100%), Changyeon Won (100%), Yizheng Wu (100%).

**Authorized Budget (BA) for FY00, FY01, FY2002:**

**FY00 BA** \$50,000

**FY01 BA** \$80,000

**FY02 BA** \$84,000

**FWP and possible subtask under FWP:** Electrode Surface Processing  
**FWP Number:** KC22

**Program Scope:**

Electrocatalysts with unique properties are created by bringing two or more different metals together as small (1 – 10 nm) bi- or multi-metallic clusters dispersed on an electronically conductive support. Various synthesis methodologies are being developed to create bi- or multi-metallic nanoclusters of a desired size, shape and composition on a well-defined substrate. In addition to high resolution electron microscopy (HRTEM), a new specialized STM/AFM technique is used to explore the surface morphology, size and shape of the bi(multi)metallic clusters, and the spatial atomic arrangement within the cluster. Monte-Carlo simulations of the bimetallic nanoclusters are conducted. The relation between electrocatalytic function and microstructural characteristics is being established.

**Major Program Achievements (over duration of support):**

Shown that non-equilibrium bimetallic surface structures produced either by ion-implantation or by electrodeposition cannot be sustained during use as a polymer electrolyte membrane (PEM) fuel cell catalyst. Sn implanted into Pt, Rh or Pd enhances the activity of the substrate for the electrooxidation of CO with a maximum effect at a surface concentration of 25 at% in all three cases. 2-5 nm bimetallic particles of Pt-Sn do not have the ordered L1<sub>2</sub> ordered structure seen in larger (> 10 nm) particles. 2-5 nm bimetallic particles of Pt-Ru do not appear to have the surface enrichment of Pt observed in the bulk crystal. Bimetallic structures unique to nanoparticles appear to be the norm rather than the exception.

**Program impact:**

A wide composition range for carbon supported bimetallic electrocatalysts must be employed to determine the optimum structure-composition. Commercial catalyst suppliers found enhanced activity after trying a wider range of compositions of Pt-Ru. Further optimization of Pt-based electrocatalysts appears possible with improved understanding of the properties of bimetallic nanoparticles.

**Interactions:**

Michel Van Hove (Monte-Carlo simulation)  
Charles Fadley (Photoelectron diffraction)  
University of the Negev (Prof. Michel Pollak)  
M.P.I. Muelheim (H. Boennemann)  
University of Bonn (Prof. Klaus Wandelt)  
Johnson-Matthey (David Thompsett)  
Tanaka Kikinzoku Kogyo (Tomoyuki Tada)

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Humbolt Foundation Fellowship (2002-04) to Matthias Arenz  
Invited Talks: Plenary Lecture at Electron Microscope Society (EMSA) Meeting by M. Radmilovic, August, 2002;  
Lecture at the Gordon Research Conference on Fuel Cells by N. Markovic, July, 2001

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

Philip Ross (P.I.) 20 %  
Nenad Markovic 33 %  
Michel Van Hove 10 %  
M. Radmilovic 20 %  
Matthias Arenz 100 % time to this project with partial support from Humbolt Foundation  
Simun Mun 50 %

**Authorized Budget (BA) for FY00, FY01, FY02:**

FY00 BA \$269,000                      FY01 BA \$271,000                      FY02 BA \$249,000

**FWP and possible subtask under FWP:** Studies of the Metal/Solution Interface

**FWP Number:** KC22

**Program Scope:**

Research is conducted to determine the structure and bonding at the metal/solution interface. Surface x-ray scattering (SXS) is used to obtain complete structural characterization of the interfacial region *in-situ* including both ions in the double layer and metal atoms at the surface. Sum frequency generation (SFG) is used to complement SXS both for the study of systems lacking long-range order, and to obtain more specific chemical bonding information. Topics under study include the structure of solvated ions at the interface, the structure of discharged or partially discharged ions on the metal surface, adsorption sites/geometries of neutral molecules adsorbed on the metal surface, and potential-dependent metal surface reconstruction/relaxation phenomena.

**Major Program Achievements (over duration of support):**

Developed new *in-situ* methodologies for structure determination at the metal/solution interface, specifically surface x-ray scattering (SXS) and vibrational spectroscopy by sum frequency generation (SFG). Investigations have focussed on structural phenomena at electrified interfaces that are especially interesting with respect to current theory. Potential driven reconstruction of Au(hkl) surfaces in solution shown to be related to charge at the surface and accounted for theoretically using a "gluon" Hamiltonian. Chloride and bromide ions shown to act as "surfactants" in the electrodeposition of Cu. Defects in Pt(hkl) surfaces shown to be responsible for nucleation of OH<sub>ad</sub> and for the oxidation of CO at low overpotentials. The structure of acetone molecules was shown to be a function of water content, nature of the cation, and the surface charge as expected from the classical Watts-Tobin theory of the double-layer.

**Program impact:**

Methodology developed in our group for in-situ SXS at the metal/solution interface being adopted by numerous groups around the world. Improved understanding of the role of chloride ion in Cu electrodeposition used by IBM to improve the model of superfilling in on-chip metallization.

**Interactions:**

University of Liverpool (Prof. Chris Lucas)

University of Cardiff (Prof. Gary Attard)

University of Bonn (Prof. Klaus Wandelt)

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

David C. Grahame Award in Physical Electrochemistry to Philip Ross (1999)

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

Philip Ross (PI) 20 %

Nenad Markovic 33 %

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$157,000

**FY01 BA** \$178,000

**FY02 BA** \$164,000

**Laboratory Name:** Lawrence Berkeley  
National Laboratory  
**B&R Code:** KC020202

**FWP and possible subtask under FWP:**

Femtosecond Dynamics in Condensed Matter

**FWP Number:** MSD KC22

**Program Scope:**

This research program is focused on understanding fundamental electronic and structural dynamics in condensed matter. Electronic excitation, vibrational excitation, scattering, relaxation, and dephasing phenomena in novel solid-state systems and molecules are investigated on the 10 fs time scale using femtosecond pump-probe, photon echo, and transient anisotropy measurements with visible pulses. Structural dynamics, atomic rearrangement, and the making and breaking of chemical bonds in condensed matter are directly investigated using time-resolved diffraction and spectroscopy techniques femtosecond x-ray pulses. The fundamental time scale for such structural phenomena is a single vibrational period, ~100 fs.

**Major Program Achievements (over duration of support):**

This research program has demonstrated that carrier scattering and dephasing dynamics in semiconductors (bulk, quantum-well, and nanocrystals) is strongly dependent on the degree of quantum confinement. In semiconductor nanocrystals, the polarization dephasing times (homogeneous linewidths) are mediated primarily by deformation coupling to acoustic modes. This coupling is strongly enhanced by the quantum confinement and is therefore size-dependent. Our research has shown that electronic and vibrational dynamics of solvated molecules is strongly influenced by both steric and dielectric interaction with the solvent environment. The nature of the coupling to the solvent bath modes is manifest in the non-Markovian behavior in the dephasing of the optical polarization. In charge-transfer systems, steric interaction with the first solvent shell mediates the speed of the reaction. Our research has further demonstrated that fundamental chemical reactions (e.g. charge transfer reactions in organo-metallic molecules and isomerization reactions in rhodopsin chromophores) are nearly barrierless transitions that proceed along non-adiabatic potentials. Excited state dynamics in the Franck-Condon region play a critical role in determining the photophysical properties of these systems. These results suggest a new paradigm for such ultrafast reactions in which the reaction proceeds from a vibrationally coherent (non-thermalized) excited state. Finally, time-resolved x-ray diffraction studies in laser-heated semiconductors have revealed the first direct evidence of non-thermal melting.

**Program Impact:** This program has elucidated a number of fundamental electronic and atomic dynamics in condensed matter systems that ultimately influence the material properties and functionality. The dynamics are inherently ultrafast due to the short interaction lengths arising from the solid density.

**Interactions:**

Internal—NERSC, Advanced Light Source, Accelerator and Fusion Research (Center for Beam Physics)

External—U.C. Berkeley Chemistry Department (A.P. Alivisatos, R. Mathies), U.C. Berkeley Physics Department (A. Zettle), Michigan State University (J. McCusker), U. Rochester Chemistry Department (S. Mukamel)

**Recognitions, Honors and Awards (at least in some part attributable to support under this program):**

C.V. Shank - John Scott Award (Franklin Society, 1991)

R.W. Schoenlein – Adolph Lomb Medal (Optical Society of America, 1992)

R.W. Schoenlein – Klaus Halbach Award (Advanced Light Source, 1996)

C.V. Shank - George E. Pake Prize (American Physical Society, 1996)

C.V. Shank - Arthur L. Schawlow Prize in Laser Science (American Physical Society, 1997)

C.V. Shank - Charles H. Townes Medal (Optical Society of America, 2001)

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

C.V. Shank, PI. R.W. Schoenlein (50%), A. Cavalleri (50%)

**Authorized Budget (BA) for FY00, FY01, FY2002:**

**FY00 BA \$284,000**

**FY01 BA \$296,000**

**FY02 BA \$272,000**

**FWP and possible subtask under FWP:**

Experimental Solid State Physics and Quantum Electronics

**FWP Number:** KC22

**Program Scope:** Development of novel nonlinear optical spectroscopic techniques to study materials and explore new areas of material science. Sum-frequency vibrational spectroscopy, for example, is developed as a surface-specific tool and used to study polymer interfaces, liquid/liquid interfaces, water/oxide interfaces, surface reactions, electrochemical interfaces, molecular conformation in molecular electronics, biomolecules adsorbed at interfaces, and molecular chirality.

**Major Program Achievements (over duration of support):**

Established the field of surface nonlinear optics by work on surface-enhanced nonlinear optical effects, nonlinear optics with surface waves, and surface second-harmonic and sum-frequency generation. Developed second-harmonic and sum-frequency spectroscopy into a powerful and versatile technique for studies of surfaces and interfaces. Successfully demonstrated unique applications of the technique to many surfaces and interfaces such as those of liquids, polymers, ice, and other solids, as well as surface reactions under ambient conditions; obtained fundamentally interesting, but hitherto unavailable, results on such interfaces. Also developed a new powerful optical technique to study surface chemical diffusions of atoms and molecules that allows sensitive probing of anisotropy, concentration dependence, impurity effect, etc. in surface diffusion. Development of sum-frequency generation as a sensitive spectroscopic tool to probe molecular chirality and study chiral biological molecules *in situ* is in progress.

Earlier work on laser/molecular beam interaction in collaboration with Y. T. Lee provided basic understanding on infrared multiphoton dissociation of polyatomic molecules.

**Program Impact:**

Developed novel laser techniques that have attracted interest of material science and chemical physics communities. Created a new research area of surface nonlinear optics in quantum electronics and surface science. The surface nonlinear optical spectroscopy technique developed in our laboratory has been adopted worldwide by many surface science groups. Our setup served as a prototype for several commercial systems.

**Interactions:**

Internal: Mat. Sci. Div. M. Salmeron, G. A. Somorjai, P. Yang; Earth Sci. Div. (G. Waychunas)

External: Inst. of Atomic and Molecular Sci., Acad. Sinica, Taiwan (M. Hayashi, S. H. Lin); Univ. Calif. at Los Angeles, Chem. Dep't (J. Heath); Wietzmann Inst. (L. Leiserowicz); Naval Res. Lab. (D. Shenoy); Univ. Hokkaido, Japan (S. Ye, K. Uosaki).

**Recognitions, Honors, and Awards**

C. H. Townes Award, Opt. Soc. Am., (1986); A. L. Schawlow Prize, Am. Phys. Soc., (1992); Distinguished Traveling Lecturer, Laser Sci. Group of APS (1994-96); Max Planck Int. Research Award (1996); Chancellor's Prof. at Berkeley (1997-2000); Mat. Sci. Award in Sol. St. Phys., Significant Implication for DOE Related Technology (1997); D. Sc. Honoris Causa, Hong Kong Univ. of Sci. and Tech., HK, (1997) and Nat. Chao Tung Univ., Taiwan (1998); F. Isakson Prize, APS (1998); Member, Nat. Acad. of Sci (1995), Amer. Acad. of Arts and Sci. (1990), Acad. Sinica (1990), Foreign member, Chinese Acad. of Sci. (1996). ); Approx. 28 invited talks plus 4 plenary talks in the last two years.

**Personnel Commitments for FY2001 to Nearest  $\pm 10\%$**

Y. R. Shen, (Group leader) 50%; M. Belkin (Student) 50%; J. McGuire (Student) 50%; Ji Na (Student), 50%, partly paid by UC; L. Zhang (Student) 50%; S-H Han (Visiting scientist) 100%, partly supported by Korea Foundation; F. Lagugne-Laparthet (Visiting scientist) 100%, supported by French CNRS; C. Zhang (Visiting scientist) 100%.

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$371,000

**FY01 BA** \$373,000

**FY02 BA** \$343,000

**FWP and possible subtask under FWP:** Center for X-Ray Optics subtask of Condensed Matter Physics  
**FWP Number:** KC23

**Program Scope:** The Center for X-Ray Optics (CXRO) pursues core programs to address national needs in the technical areas of high-spatial and high-spectral resolution applications of electromagnetic radiation in the soft x-ray and extreme ultraviolet regions of the spectrum. Additionally, CXRO builds and uses systems/instruments in this region for a wide range of scientific and technological applications in collaboration with other organizations. Elements of the program consist of ultra high-resolution x-ray microscopy/tomography, spectroscopy, interferometry, Fourier optics, techniques of modern optics, and x-ray coherence measurement, generation, and theory. Additionally, CXRO has developed significant nanofabrication expertise to support experimental activities.

**Major Program Achievements (over duration of support):**

CXRO continued the development and implementation of an x-ray microscope with the world's highest resolution diffractive optics, resolving 21nm half pitch lines and spaces, for two and three-dimensional (tomographic) studies of magnetic materials, electromigration, life sciences samples, and environmental/remediation. CXRO developed innovative optics for x-ray absorption, phase shifting measurements of f1 and f2 scattering factors using diffractive optics and interferometry. CXRO has pioneered the study of and developed new applications of the coherence properties of synchrotron and non-synchrotron radiation. CXRO has designed and constructed a new undulator beam-line dedicated to coherent science including the coherent x-ray scattering from partially ordered materials systems, such as magnetic and superconducting materials, to study the static and dynamic behavior of these systems.

**Program Impact:**

Since being established in 1983, CXRO has been a world leader in the development and applications of high-resolution x-ray optics, including nanofabrication of diffractive optics. X-ray microscopy studies of magnetic materials are having an impact on the understanding of complex and technologically significant material interactions. Studies of copper and tungsten electromigration have shown mechanisms of void formation along grain boundaries that are significant for Integrated Circuit reliability. X-ray microscopy-tomography studies of cells have generated sufficient interest at NIH that a large NIH funded user program is an excellent possibility. Scattering coefficients (both real and imaginary) have been measured with high-accuracy near absorption edges using a new interferometric technique have impacted phase shift mask design for EUV lithography. The CXRO maintained database of scattering factors, available online, is heavily used by researchers throughout the world.

**Interactions:**

CXRO has numerous interactions with university, national laboratories, and industry, including: U. Colorado, Colorado State, U. Oregon, U. Washington, Stanford, U. Wuerzburg, U. Gottingen, UCSF, LLNL, Sandia, Argonne, Intel, HP, Shipley, IBM, AMD, Motorola, Max Planck

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

**Personnel Commitments for FY2002 to Nearest +/-10%:**

Scientific Staff	FTE
Erik <b>Anderson</b>	0.1
Dave Attwood	0.2
Greg Denbeaux	1.0
Eric Gullikson	0.3
Keith Jackson	0.2
Alex Liddle	0.1
Stan Mrowka	0.1
Angelic Pearson	1.0
Rupert Perera	0.7

Matrix Labor	FTE
Engineering	1.0
Technician	3.0
CSE & Programming	1.2

**Authorized Budget (BA) for FY00, FY01, FY02:**

FY00 BA \$ 1,953,000

FY01 BA \$ 2,046,000

FY02 BA \$ 1,851,000

**FWP and possible subtask under FWP:** Quantum Theory of Materials  
**FWP Number:** KC23

**Program Scope:** Theoretical calculations are employed to further the basic understanding of the physical properties of materials and materials systems. The emphasis is on carrying out quantum-mechanical calculations for realistic systems based on microscopic first-principles approaches. Model systems are also examined, and new theoretical techniques are developed. Studies include bulk materials, fullerenes, nanotubes, superconductors, surfaces and chemisorbed systems, materials under high pressure, two-dimensional electron systems, polymers, clusters, and defects in solids. Close collaboration with experimentalists is maintained.

**Major Program Achievements (over duration of support):** Explained properties of materials (e.g., bonding and structural properties; band structure and optical properties; properties of defects, surfaces, clusters and nanostructures) and predicted new materials and phenomena (e.g., superhard materials, new class of compound nanotubes, new phases of materials under high pressures, new superconductors). Developed theoretical and computational methods (e.g., the empirical and ab initio pseudopotential methods, supercell technique, total energy method for structural properties, many-body Green's function approaches for spectroscopic properties, and quantum Monte Carlo method for electron correlation effects.) Most recent highlights include calculations of electronic and transport properties of nanostructures, solid-state NMR spectra, multigap superconductivity in MgB<sub>2</sub>, optical properties of surfaces and polymers, and ideal strength of materials.

**Program Impact:** Led to new discoveries, explanation of experiments, and development of methods. Advances of major impact include systematic unraveling of optical and photoemission properties of semiconductors; determination of surface/interface structures and properties; calculation and prediction of structural phase transitions; solution to the band gap problem; quantum Monte Carlo studies of real materials; prediction of superconductivity, superhard materials and new nanotubes. The theoretical and computational methods (discussed above) developed have become standard tools in the field and are being used by theory groups worldwide. Many of the former students and postdocs of the program are now leaders in the field in academia, industry and national laboratories.

**Interactions:**

Internal—NERSC/LBNL (Canning, Wang), MSD/LBNL (Zettl, Crommie)

External—University of Minnesota; University of Washington; Palo Alto Research Center; LLNL; Georgia Tech

International—Grenoble High Magnetic Field Lab; Tokyo Institute of Science; Seoul National University; Korea Advanced Institute of Science; Taiwan National Center for Theoretical Science; IU. Pais Vasco (UPV/EHU), Spain.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

**M. L. Cohen** – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; APS Buckley Prize; DOE Outstanding Accomplishment in Solid State Physics Award; DOE Sustained Outstanding Accomplishment in Solid State Physics Award; APS Lilienfeld Prize; U.S. National Medal of Science; ISI's top 100 most-cited physicists; 25 invited talks since 2000.

**S. G. Louie** – Fellow of APS; Sloan Fellow; Guggenheim Fellow; DOE Sustained Outstanding Research in Solid State Physics Award; APS Aneesur Rahman Prize; APS Davisson-Germer Prize; ISI's top 100 most-cited physicists; 45 invited talks since 2000.

**Personnel Commitments for FY2002 to Nearest +/-10%:**

M.L. Cohen (25%); S.G. Louie (25%); C. Spataru (50%); W. Luo (50%); H. J. Choi (50%, fellowship); H. Sun (50%, fellowship); F. Ribeiro (50%); W. Duan (50%, fellowship)

**Authorized Budget (BA) for FY00, FY01, FY02:**

FY00 BA \$268,000

FY01 BA \$268,000

FY02 BA \$238,000

**FWP and possible subtask under FWP:**  
Low-Temperature Properties of Materials

**FWP Number:** KC23, KC31

**Program Scope:**

Specific-heat measurements, including measurements under pressure and in magnetic fields, are used to investigate relations between chemical composition, structure, and physical properties. One area of emphasis is magnetic materials and superconductors, including the interplay between magnetism and superconductivity in heavy-fermion compounds; another is the use of small-sample techniques to study materials available only in small quantities, including nanoparticles and carbon nanotubes.

**Major Program Achievements (over duration of support):**

The melting of the vortex lattice in YBCO has been shown to change from first order to second order at a critical pressure at which a second liquid phase appears. The ferromagnetic ordering in “colossal-magneto-resistance” (La,Ca)MnO<sub>4</sub> is thermodynamic first-order in zero magnetic field, but changes dramatically in small fields; the O isotope effect is large, unusual, and field dependent. The existence of line nodes in the energy gaps of YBCO and (La,Sr)CuO<sub>4</sub> has been demonstrated. MgB<sub>2</sub> was shown to be a “two-gap” superconductor, and the gap parameters determined. With increasing pressure the nature of the magnetic ordering in antiferromagnetic CeRhIn<sub>5</sub> changes continuously, but there is a discontinuous change in the ground state and a weak first-order transition at the critical pressure at which superconductivity appears; the superconductivity evolves from gapless to fully gapped with increasing pressure; the order parameter is “unconventional”. Thermodynamic features in the phase diagram of the ferromagnet/superconductor UGe<sub>2</sub> have been identified. Preliminary measurements on Pd nanoparticles have shown the feasibility of measurements on nanoparticles as prepared at LBL.

**Program impact:**

The recognition of the second liquid phase in the “vortex matter” of YBCO is the first experimental evidence of a new, theoretically predicted transition. The measurements on (La,Ca)MnO<sub>4</sub> have determined the thermodynamic nature of the magnetic ordering in zero field, shown that much of the magnetic entropy is recovered at higher temperatures, defined the nature of the low-temperature ground state, and given new constraints on theoretical models of the magnetic ordering. The measurements on YBCO and (La,Sr)CuO<sub>4</sub> have added to the evidence of a d-wave order parameter in the high-T<sub>c</sub> cuprate superconductors. MgB<sub>2</sub> is the first really “clean” example of a multiband superconductor and shows effects that were first predicted 30 and 40 years ago. The pressure-induced transition to superconductivity in CeRhIn<sub>5</sub> is different from that in other Ce heavy-fermion compounds, underlining the limitations on current theoretical understanding of the relation between magnetism and superconductivity in these materials.

**Interactions:**

Internal: P. Alivisatos; A. Zettl; M. Cohen; S. Louie. External: ANL; LANL; Max Planck Institute: Centre Etude Nucleaire Grenoble; University of Alberta; Amherst College.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Invited talks: M<sup>2</sup>S HTSC, Houston 2000 (2); APS March Meeting, 2000; APS March Meeting, 2001; SCRM, Giens, France, 2002; ASR, Tokai, Japan, 2002.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

N. E. Phillips, 100% on project, paid ~25%; R. A. Fisher, ~50% on project, paid ~25%; N. Oeschler, starting date uncertain, 100%.

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$173,000

**FY01 BA** \$173,000

**FY02 BA** \$157,000

**Laboratory Name:** Lawrence Berkeley  
National Laboratory  
**B&R Code:** KC020203

**FWP and possible subtask under FWP:**

Femtosecond X-ray Beamline for Studies of Structural Dynamics

**FWP Number:** MSD KC23

**Program Scope:**

The application of x-ray techniques to study ultrafast structural dynamics such as phase transitions, chemical reactions, and surface processes on the fundamental time scale of a vibrational period (~100 fs) is an important new field of research in physics, chemistry, and materials science. The objectives of this research program are: (1) to develop a state-of-the-art research facility for time-resolved x-ray science based on a synchrotron beamline generating 100 fs x-ray pulses, (2) to develop scientific applications and associated measurement techniques utilizing femtosecond x-ray pulses, and (3) to provide scientific support for beamline users in the area of time-resolved x-ray science.

**Major Program Achievements (over duration of support):**

This research program has provided the first demonstration of femtosecond pulses generated from a synchrotron. The femtosecond x-ray flux and background levels have been characterized and compared with model calculations. This research program has supported the development of a bend-magnet beamline and instrumentation at the ALS for time-resolved measurement including a sub-picosecond x-ray streak camera with photoconductive trigger. Finally, this program provides scientific support of user research using time-resolved x-ray techniques.

**Program Impact:**

This program is a leading contributor to the development of the new research area of femtosecond x-ray science.

**Interactions:**

Internal - LBNL Chemical Sciences Division (A. Belkacem, M. Prior), Advanced Light Source, LBNL Accelerator and Fusion Research Division (Center for Beam Physics)

External - U.C. Berkeley Physics Department (R. Falcone), Michigan State University (J. McCusker), Univ. of Lausanne (M. Chergui, C. Bressler).

**Recognitions, Honors and Awards (at least in some part attributable to support under this program):**

R.W. Schoenlein – Klaus Halbach Award (Advanced Light Source, 2000)

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

R.W. Schoenlein (50%), A. Cavalleri (50%)

**Authorized Budget (BA) for FY00, FY01, FY2002:**

**FY00 BA \$0**

**FY01 BA \$287,000**

**FY02 BA \$272,000**

**Laboratory Name:** Lawrence Berkeley National Laboratory

**B&R Code:** KC020301

**FWP and possible subtask under FWP:** Physical Chemistry of Nanocrystals

**FWP Number:** KC31

**Program Scope:** Nanometer size inorganic crystals are playing an increasingly important role in solid-state physics, chemistry, materials science, and even biology. Many fundamental properties of a crystal (e.g., ionization potential, melting point, band gap, saturation magnetization) depend upon the solid being periodic over a particular length scale, typically in the nm regime. By precisely controlling the size and surface of a nanocrystal, its properties can be tuned. Using techniques of molecular assembly, new nanocrystal-based materials can in turn be created. This program encompasses fundamental studies of the mechanisms and kinetics of nanocrystal synthesis as well as studies of scaling laws for optical, electrical, magnetic, and structural size dependent properties.

**Major Program Achievements (over duration of support):** Helped develop the concept of inorganic nanocrystals as a class of macromolecule. First studies of surface derivitization and isolation of nanocrystals, and immobilization of nanocrystals on self-assembled monolayers; first photoelectron spectroscopy studies of nanocrystal electronic structure (with Jim Tobin) and nanocrystal surface structure. Development of X-ray Absorption Spectroscopy as a tool for determining nanocrystal surface structure; first measurements of single nanocrystal x-ray absorption spectra. Synthesis and shape control of semiconductor nanocrystals and nanorods of CdSe, InP, InAs, GaAs, Co, and Fe<sub>2</sub>O<sub>3</sub>. Discovery of branching in nanorod synthesis of II-VI semiconductors, including synthesis of tetrapods and inorganic dendrimers. Studies of core-shell nanocrystal synthesis and properties. Optical properties of nanocrystals, including hole-burning, resonance Raman, photon echo, Stark effect; polarization and blinking studies of quantum dots and nanorods. Studies of pressure and temperature induced structural transformations in nanocrystals. These studies have shown that the kinetics of structural transformations are better defined in nanocrystals than in bulk solids, processing by well-defined pathways. Phenomena discovered include single nucleation events in nanocrystal structural transformations; shape change as an indicator of mechanism in nanocrystal transformations, first measurements of activation energy and activation volume in nanocrystal structural transformations. First electrical device based on a nanocrystal-polymer composite (light emitting diode); first transistor based on a single nanocrystal and a single molecule (with Paul McEuen); developed the use of DNA as a tool for patterning nanocrystals (with Peter Schultz); discovered liquid crystal phases of semiconductor nanorods; introduced the use of colloidal quantum dots as fluorescent biological labels (with Shimon Weiss); Hybrid nanorod-polymer solar cell.

**Program impact:** Light emitting diodes, solar cells, solar concentrators, fluorescent biological labels (reduced photobleaching, multiplexed assays), magnetic storage, magnetic bio-labeling, mechanical reinforcement of composites. Education: About 100 scientists have been trained in the lab, and are now active in the science community. (alumni at Arkansas, Bain Consulting, Exxon-Mobil, General Electric, Univ. of Hamburg, Harvard, Hebrew Univ. of Jerusalem, Univ. of Mainz, MIT Media Lab, Mitsubishi Chemical, Nanotectonica, Naval Research Lab, Patent Attorney, Quantum Dot Corp., Rice, National Taiwan University, Siemens, UCLA, Vanderbilt).

**Interactions:** Current collaborators: Jean Frechet (Chemistry and MSD), Daniel Chemla (Physics and MSD), Alex Pines (MSD and Chemistry), Anupam Mahukar (USC), Ned Seeman (NYU), Laura Landweber (Princeton), Priya Vashista (LSU), Lydia Sohn (Princeton). Former collaborators: Chuck Shank, Peter Schultz, Paul McEuen. Industry Interactions: Founder, Quantum Dot Corporation; Founder, Nanosys, Inc. Consulting: 3M, Dow Chemical, Dupont, Intel, Kodak, Motorola, Xerox; Bayer, BASF, Mitsubishi Chemical, Samsung.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):** Ten issued. Founded two companies: Quantum Dot Corporation (fifty employees) with focus on biomedical applications of semiconductor nanocrystals, and most recently, Nanosys, with focus on electro-optic applications. Press Articles: C&E News, Science, Nature, Science News, Scientific American, MIT Technology Review, Red Herring, Business Week, Service to the community: Founding editor-in-chief of Nano Letters (American Chemical Society); Associate Editor, Annual Reviews of Physical Chemistry; co-author with Mike Roco of the NSF and Stan Williams of HP, of the National Nanotechnology Initiative Report. DOE Council on Materials Science; External Review Board of the Joint Institute of Laboratory Astrophysics; National Research Council Solid State Sciences Subcommittee. Examples of Awards and Honors: ~30 plenary and invited lectures last year, including seven endowed lectureships; NSF Presidential Young Investigator, Sloan Foundation Fellow, Exxon American Chemical Society Solid State Chemistry Fellowship, Materials Research Society Outstanding Young Investigator, Wilson Prize, Harvard University, Fellow of the American Physical Society, Fellow of the American Association for the Advancement of Science, Visiting Professor St. John's College Cambridge.

**Personnel:** Paul Alivisatos (PI), 12 graduate students, 8 postdoctoral fellows, many visitors

**Authorized budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$472,000

**FY01 BA** \$475,00

**FY02 BA** \$433,000

**Laboratory Name:** Lawrence Berkeley National Laboratory

**B&R Code:** KC020301

**FWP and possible subtask under FWP** Self-assembly of organic/inorganic nanocomposites materials

**FWP #:** KC31

**Program Scope:** The goal is to design functional materials and make them by parallel and hierarchical self-assembly. In particular, we seek to develop wet chemical processes by which organic/inorganic composites can be created with a high degree of control on many length scales simultaneously. By developing a comprehensive ability to pattern organic/inorganic composites, it will be possible to design complex materials in which several microscopic processes are independently and simultaneously optimized. A range of functional materials can be created in this manner, with applications in energy conversion, mechanical composites, and optical/electrical devices. The team consists of Paul Alivisatos (inorganic nanocrystals); Jean Frechet (Polymers and Organic Synthesis); Miquel Salmeron (Spectromicroscopy and Imaging); and Lin Wang Wang (Theory).

**Major Program Achievements (over duration of support):** Demonstrated the concept of hybrid inorganic-organic nanorod – polymer solar cells (Science 2002, 295, 2425.); developed new specialty electro-active surfactants that solubilize inorganic nanorods, while permitting electron transfer (Adv. Mater., in press); calculated the energy levels of semiconductor nanorods vs. aspect ratio, and verified the prediction that the degree of polarization should change dramatically at aspect ratio of 2 (Science 2001, 293, 1455, Journal of Physical Chemistry B 2002, 106, 2447); discovered the existence of liquid crystal phases of inorganic semiconductor nanorods (Nano Letters 2002, 2, 557.). Currently in press: computed the energy levels of exotically shaped nanocrystals – arrows and teardrops; demonstrated the synthesis in high yield of branched nanocrystals; demonstrated the growth of nanocrystals by microfluidic techniques; demonstrated solution phase X-ray absorption spectroscopy of Co nanocrystals; AFM investigations of inorganic tetrapods.

**Program Impact:** Examples of Applications: hybrid nanorod – polymer solar cells; light emitting diodes; mechanical reinforcement of plastics. Education: About 100 scientists have been trained in the lab, and are now active in the science community. (alumni at Arkansas, Bain Consulting, Exxon-Mobil, General Electric, Univ. of Hamburg, Harvard, Hebrew Univ. of Jerusalem, Univ. of Mainz, MIT Media Lab, Mitsubishi Chemical, Nanotectonica, Naval Research Lab, Patent Attorney, Quantum Dot Corp., Rice, National Taiwan University, Siemens, UCLA, Vanderbilt). Patents: Ten issued. Founded two companies: Quantum Dot Corporation (fifty employees) with focus on biomedical applications of semiconductor nanocrystals, and most recently, Nanosys, with focus on electro-optic applications. Press Articles: C&E News, Science, Nature, Science News, Scientific American, MIT Technology Review, Red Herring, Business Week Service to the community: Founding editor-in-chief of Nano Letters (American Chemical Society); Associate Editor, Annual Reviews of Physical Chemistry; co-author with Mike Roco of the NSF and Stan Williams of HP, of the National Nanotechnology Initiative Report. DOE Council on Materials Science; External Review Board of the Joint Institute of Laboratory Astrophysics; National Research Council Solid State Sciences Subcommittee.

**Interactions:** Current team members: Paul Alivisatos (Chemistry and MSD) Jean Frechet (Chemistry and MSD), Miquel Salmeron (MSD); LinWang Wang (NERSC); Collaborators: Richard Mathies (Chemistry) (Daniel Chemla (Physics and MSD), Alex Pines (MSD and Chemistry), Anupam Mahukar (USC), Ned Seeman (NYU), Laura Landweber (Princeton), Priya Vashista (LSU), Lydia Sohn (Princeton). Former collaborators: Chuck Shank, Peter Schultz, Paul McEuen. Industry Interactions: 3M, Dow Chemical, Dupont, Intel, Kodak, Motorola, Xerox; Bayer, BASF, Mitsubishi Chemical, Samsung.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):** Alivisatos: ~30 plenary and invited lectures last year, including seven endowed lectureships; NSF Presidential Young Investigator, Sloan Foundation Fellow, Exxon, ACS Solid State Chemistry Fellowship, MRS Outstanding Young Investigator, Wilson Prize, Harvard, Fellow APS, Fellow AAAS, Visiting Professor St. John's College Cambridge. Fréchet: NAS, NAE, AAAS; ACS Award n Polymer Chemistry, Butler Lecturer Florida, ACS Salute to Excellence Award, ACS Cope Scholar Award, Baker Lecturer Cornell, Stauffer Lecturer Stanford, Bayer Lecturer, Pittsburgh, Chute Lecturer Dalhousie, Merk-Frosst Lecturer Alberta, Chambers Lecturer Rochester, Dow Karabatos Lecturer Michigan State, Doctorate (Honoris Causa) Université Claude Bernard, France. Salmeron: Plenary lecturer 18<sup>th</sup> European Conf. on Surface Science, Keynote speaker 1<sup>st</sup> Latin American Sym. on Scanning Probe Microscopy. 13 invited talks since 2001.

**Personnel Commitments for FY2002 to Nearest +/-10%:** Paul Alivisatos (PI), 12 graduate students, 8 postdoctoral fellows, many visitors

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA \$0      FY01 BA \$1,600,000      FY02 BA \$1,459,000**

**FWP and possible subtask under FWP:** Biomolecular Materials Program

**FWP Number:** KC31

**Program Scope:** Study of the mimicking or application of biological materials and processes in the materials sciences. Current studies include the mimicking of membranes and membrane receptors for coatings and functional interactions with living cells; of carbohydrates for controlled interface properties; of proteins for nanoscale conducting wires and self-assembling building blocks for functional assemblies; of DNA and dendrimers for 3-D patterning of inorganic nanocrystals, and as components of functional assemblies; of antibodies and molecular recognition elements (in collaboration with John Clarke) for ultrasensitive biosensors;

**Major Program Achievements (over duration of support):** Development of biosensors that turn color in the presence of agents such as influenza virus, botulinum toxin(Charych). Development of ultrasensitive SQUID based biosensors that respond for pathogens (Alper/Clarke). Development of polymers that significantly improve the stability of proteins in unbuffered solutions and at elevated temperatures (Bednarski). Development of catalytic antibodies (Schultz). Development of systems to insert non-natural amino acids into proteins (Schultz). Exploration of the effect of specific amino acid substitutions on proteins temperature stability (Kirsch). Discovery of enzyme mechanisms for discrimination between optical isomers.(Koshland). Development of techniques to metabolically modify cells for specific attachment to inorganic surfaces without loss of function (Bertozzi). Development of techniques for the use of DNA and polymers for the spatial arrangement of nanocrystals. Development of a new approach for mineralizing organic polymer surfaces with inorganic composites for tough, lightweight, fracture-resistant organic/inorganic hybrid materials modeled on bone (Bertozzi). Development of new biomimetic, carbohydrate-like polymers with lubricating properties.modeled after biological mucins (Bertozzi). Development of methods for isolating gold nanocrystals bearing discrete numbers of DNA oligonucleotides and the preparation of dimers and trimers of these DNA-nanocrystal assemblies and a wide variety of other spatial arrangements of nanocrystals (Alivisatos). Development of a series of unnatural building blocks to enable automated preparation of self-assembling dendritic materials based on DNA base pairing (Frechet). Preparation of well defined assemblies of nanocrystals in specific arrangements (Frechet). Development of a system to deliver biological molecules to prepatterned membrane structures using targeted membrane fusion (Groves). Modification of two natural products to allow their attachment to inorganic surfaces to direct actin polymerization in rudimentary circuits. Attachment of polymers and other molecules to the viral coat protein as building blocks for complex structures.

**Program Impact:**

Developed biosensors for study by industry and government for military and civilian use. Expanded the capability to specifically modify enzymes to perform novel functions. Commercial product for the stabilization of proteins at high temperatures and in unbuffered solutions. Developed techniques for creating hybrid devices of living cells and non-living materials. Published in excess of 10 papers/year in major peer reviewed journals.

**Interactions:**

C. Larabell, UCSF; L. Landweber, Princeton; N. Seeman, NYU; M. Dustin, NYU; M. Callstrom, Ohio State Univ.; A. Tomsia, R. Ritchie, K. Healy, R. Mathies, E. Isacoff, LBL and UCB.

**Recognition, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Bertozzi-Irving Sigal Young Investigator Award of the Protein Society, ACS Award in Pure Chemistry, Merck Academic Development Program Award, Presidential Early Career Award in Science and Engineering, MacArthur Foundation Award, Camille Dreyfus Teacher-Scholar Award, Arthur C. Cope Scholar Award ACS Alivisatos-Fellow, AAAS, APS, Wilson Prize- Harvard, Coblentz Award, Sloan Foundation Fellow, Presidential Young Investigator, Outstanding Young Investigator-MRS, Editor-in-Chief NanoLetters, Associate Ed. Ann Rev Phys Chem, Editorial Board: J Phys Chem, Chem Phys, J Chem Phys (APS) Frechet-Nat. Acad Sci, Nat Acad Engin, Amer Acad Arts and Sci, ACS Award in Polymer Chem, ACS Salute to Excellence Award, ACS Cope Scholar Award, Baker Lecturer-Cornell, Stauffer Lecturer- Stanford, Groves- Searle Scholars Award, Francis-Dreyfus foundation award

**Personnel Commitments for FY2002 to Nearest +/-10%:**

Mark Alper, 10% , Profs. Paul Alivisatos, Jean Frechet ,Carolyn Bertozzi, Jay Groves, Matt Francis, Dr, Jie Song, Dr. Goo Soo Lee, Dr. Cathie Klapperich, Howard Hang, Christine Micheel 50%, Aihua Fu 50% , Brian Carlson, Danielle Dube, Sarah Luchansky, Sarah Goh,Michael Dubber, Dean Lee, Annapoorna Sapuri, Ernest Kovacs, Jacob Hooker, Harvey Johnson 50%, Neel Joshi50%, Amanda Crochet, Trung Nguyen, Tara Schlick 50%

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$524,000

**FY01 BA** \$593,000

**FY02 BA** \$781,000

**FWP and possible subtask under FWP:**

Polymer Program: Controlling macromolecular structure, architecture and functionality in energy related polymeric materials.

**FWP Number:** KC31

**Program Scope:**

The program seeks a fundamental understanding the synergistic relationship between macromolecular structure, sequence, architecture and functionality for energy related polymeric materials. The program includes major components in the four complementary areas of theory, synthesis, and physical as well as functional property determination. Totally novel functional polymers of potential importance to energy applications are being designed, prepared and studied. A particular emphasis concerns stimuli-responsive polymers containing elements or features that confer electroactive, thermoresponsive, pH or light responsive properties.

**Major Program Achievements (over duration of support):**

Developed theory predicting unusual properties for randomly branched copolymers. Reduced theory to practice with the preparation of a first family of randomly branched copolymers using living polymerization techniques. Carried out scattering and other property measurements on randomly branched copolymers. Developed novel synthetic approach to polymers with novel architecture including star copolymers and dendritic polymers. Studied the properties of these novel star and dendritic polymers.

Explored the potential of the novel polymers with controlled architecture for applications such as microfluidics and catalysis. Initiated the study and physical characterization of novel families of crosslinked polymers.

**Program impact:**

Novel polymers with controlled architectures have great potential as smart materials providing functional properties not achievable with more standard polymers or polymer blends. Early demonstrations of capabilities have included thermoresponsive materials that can operate as valves without moving parts, microfluidic systems and efficient catalysts.

**Interactions:**

Internal interactions: Division of Materials Sciences LBNL, Physical Biosciences Division LBNL, NCEM

External interactions: Stanford University, Sandia National Laboratory, Air Force Research Laboratories, NIST, Cornell University, City College CUNY, University of Rhode Island, Polytechnic University, New York University, Harvard University, Kyoto University, University of Athens

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

N. Balsara: Fellow of the American Physical Society 2001; Program Chair for AIChE 2002

A. Chakraborty: R.W. Vaughan Memorial Lecturer Caltech 2000; Miller Research Professor University of California, Berkeley.

S. Muller: Journal of Rheology publication award 1998

J. Frechet: National Academy of Sciences 2000, National Academy of Engineering 2000, American Academy of Arts and Sciences 2000, American Chemical Society Award in Polymer Chemistry 2000, Butler Lecturer University of Florida 2000, American Chemical Society Salute to Excellence Award 2001, American Chemical Society Cope Scholar Award 2001, Baker Lecturer Cornell University 2001, Stauffer Lecturer Stanford University 2001, Bayer Lecturer University of Pittsburgh 2001, Chute Lecturer Dalhousie University 2002, Merk-Frosst Lecturer University of Alberta 2002, Chambers lecturer University of Rochester 2002, Dow Karabastos Lecturer Michigan State University 2002, Doctorate (Honoris Causa) Universite Claude Bernard, France 2002.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

Frechet 20%, Balsara 20%, Chakraborty 20%, Muller 20%, 2 postdocs (100%), 3 students (100%)

**Authorized Budget (BA) for FY00, FY01, FY02:**

FY00 BA \$595,000

FY01 BA \$587,000

FY02 BA \$553,000

**Laboratory Name:** Lawrence Berkeley National Laboratory  
**B&R Code:** KC0203010

**FWP and possible subtask under FWP:**

FWP Microscopy Investigations of Quantum Dots, Nanorods, and Soft Condensed Matter

**FWP Number:** CHLEO0201

**Program Scope:**

Development of innovative microscopies, such as near field microscopy and CARS microscopy, to study problems in the growth of semiconductor quantum dots and nanowires, vapor uptake in soft condensed matter, and ultrafast processes in semiconductor nanostructures. This work establishes the limits of spatial and time resolution in the study of nanostructured materials.

**Major Program Achievements (over duration of support):**

New laboratories were set up and made functional. Growth of GaN has been established in a new apparatus by molecular beam epitaxy. Measurements of film growth flatness and x-ray analysis of crystal structures demonstrate that excellent quality films are produced. Photoluminescence studies of GaN have been initiated. Growth of ZnO nanowires has been successful, and luminescence from ZnO nanowires has been observed and characterized. Ultrafast laser, differential absorption experiments on ZnO material are being initiated.

**Program Impact:**

Work in polymer lithographic materials has significant impact on the semiconductor industry, related to the whole field of patterning and line dimension reduction. Studies of InGaN are important for the lighting industry and for energy efficiency.

**Interactions:**

A collaboration with IBM scientists, William Hinsberg and Frances Houle to advance the state of the art in detection of latent images in lithographic polymer films.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Invited talk, American Vacuum Society national meeting.  
Keynote lecture, Advanced Light Source User's Workshop

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

S. Leone (PI)  
T. Zhang (graduate student) 50%  
B. Liu (post-doc) 50%  
J. Szarko (graduate student) 50%  
C. Blackledge (post-doc) 100%

**Authorized Budget (BA) for FY00, FY01, FY02:**

<b>FY00</b> \$0	<b>FY01</b> BA \$0	<b>FY02</b> BA \$100,000
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**Laboratory Name:** Lawrence Berkeley National Laboratory

**B&R Code:** KC020301

**FWP and possible subtask under FWP:** Nuclear Magnetic Resonance

**FWP Number:** KC31

**Program Scope:** The nuclear magnetic resonance (NMR) program has two complementary components. The first is the establishment of new concepts and techniques in NMR and its offspring, magnetic resonance imaging (MRI), in order to extend their applicability and enhance their capability to investigate molecular structure and organization from materials to organisms. The study and diagnostic use of nuclear spins interacting with each other and with others degrees of freedom requires the development of new theoretical and experimental methods; one consequence of these efforts is the design and fabrication of next-generation NMR and MRI equipment. The second component of the research program involves the application of such novel methods, together with other programs, and with outside laboratories and industry, to significant problems in chemistry, materials science and biomedicine. It is the unique environment of interdisciplinary research and large-scale technical and instrumentation capabilities at the Lawrence Berkeley National Laboratory that cultivates these innovations and their diverse applications.

**Major Program Achievements (over duration of support):** Some principal developments: Helped launch high-resolution solid-state NMR of dilute spins in solids. Introduced multiple-quantum spectroscopy, the conceptual foundation and methodology of which are now widely used within the framework of modern multidimensional NMR in liquids and solids. Developed zero-field Fourier-transform NMR using both magnetic field cycling and superconducting detectors. Invented dynamic-angle spinning and double rotation, based on coherent averaging under icosahedral symmetry, making possible the first high-resolution NMR of quadrupolar nuclei such as oxygen-17 and aluminum-27 solids. Made advances in optical pumped and detected NMR and MRI through the combination of laser-polarized xenon with polarization transfer, and the development of novel xenon-based NMR sensors. Most recently, introduced ex-situ and remote detection of NMR and MRI, soon poised to allow external scanning of objects and subjects. Examples of novel techniques: Cross-Polarization, High-resolution Solid-State NMR, Quadrupoles, Dynamic-Angle Spinning, Double Rotation-Multiple-Pulse Schemes, Iterative Maps and Sequences, Multidimensional and Variable-Angle Correlations-Multi-Spin Systems, Multiple-Quantum Coherence, Time-Reversal, Irreversibility, Decoupling and Recoupling-Long-Range Dipolar Couplings in Liquid Crystals, Molecular Structures, Macromolecules, Quantum Computing-*Ex-Situ* High-Resolution NMR and MRI, Remote NMR and MRI, Optical Pumping and Detection, Dipolar Detector-Zero-Field NMR, Ultralow-Field NMR and MRI, J-Coupling Spectroscopy, SQUID Detection of Polarized Gases-Laser-Polarized Xenon NMR and MRI, Polarization transfer for Lighting Up NMR and MRI, Xenon Biosensor Examples of Applications: Structure and Dynamics in Porous Materials, Minerals, Catalysts, Semiconductors, Surfaces, Amorphous materials, Glasses, Nanocrystals, Nanotubes, Polymers, Biomolecules, Tissue, Organisms.

**Program impact:** Seeing is believing; novel techniques and devices of magnetic resonance spectroscopy and imaging have expanded our ability to “see” into materials and organisms. The concepts and instrumentation, adopted worldwide by laboratories and industry, are being used to investigate molecular structure and organization from the nanoscale dimensions of catalysts and polymers to the macroscopic proportions of human imaging and oil exploration. Education: More than 200 scientists (“Pinenuts”) trained in lab, many holding leading position in academia and industry. Patents: More than twenty issued, filed, pending; methodologies licensed, adapted into commercial NMR technology. Journal Covers: e.g. Science, Spectroscopy, J. Magnetic Resonance, Angewandte Chemie, J. Physical Chemistry. Press Articles: e.g. C&E News, Science, Nature, Science News, Scientific American, Biophotonics, Spectroscopy.

**Interactions:** Paul Alivisatos (MSD and Chemistry), Jeffrey Reimer (MSD and Chemical Engineering), David Wemmer (Biology and Chemistry), John Clarke (MSD and Physics), Erwin Hahn (Physics), Thomas Budinger (Bioengineering), Stanley Prusiner (UCSF), Peter Schultz (Scripps and Novartis), Allen Garroway (NRL). Industry: e.g. Varian Instruments, Amersham, Schlumberger-Doll, IBM, Shell, Exxon, Mobil, Monsanto, Du Pont.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Recognition: Glenn T. Seaborg Chair, UC Berkeley; Foreign Member, Royal Society; Scientific American “50” Visionaries; Docteur Honoris Causa Universities of Rome and Paris. Awards and Honors: e.g. National Academy of Sciences; ACS Baekeland Medal, DOE E.O. Lawrence Award; Pittsburgh Spectroscopy Award; Wolf Prize in Chemistry; Centenary Medal, Royal Society of Chemistry; ACS Irving Langmuir Award in Chemical Physics; F.S. Cotton Medal; Dickson Prize, Carnegie-Mellon university; Tetelman Fellow, Yale University; Ampere Congress in Honor of AP’s 50<sup>th</sup> Birthday; 2 R&D-100 Awards; Tech Transfer Award; UC Distinguished Teacher Award; Professeur Joliot-Curie; Ecole Supérieure, Paris; Loeb Lecturer, Harvard University; Lord Lecturer, MIT; Roberts Lecturer, Caltech, Hinshelwood Professor, Oxford University; Lord Todd Professor, Cambridge; Bircher Lecturer, Vanderbilt University; ~ 30 plenary and invited lectures last year.

**Personnel Commitments for FY2002:** Alexander Pines (PI), 16 graduate students, 8 postdoctoral fellows, many visitors.

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$748,000

**FY01 BA** \$702,000

**FY02 BA** \$938,000

**FWP and possible subtask under FWP:** Mechanical and chemical properties of surfaces and interfaces  
**FWP Number:** KC31

**Program Scope:**

Fundamental studies of surface structure, dynamics, friction, adhesion, lubrication and wear. Energy transfer in atomic scale contacts. Mechanisms of atomic scale manipulation. Development of advanced atomic scale imaging and spectroscopy techniques: Scanning Tunneling and Atomic Force Microscopies, (STM and AFM).

**Major Program Achievements (over duration of support):**

Nanotribology: Discovery of friction mechanism in monolayer lubricants due to concerted molecular tilting of alkyl chains (application in MEMS, self-assemble films). Demonstration of two-dimensional drainage of single molecular layers of lubricants, (applications to hard disk lubricants). Development of Scanning Polarization Force Microscopy, a novel technique for imaging liquid structure with nanometer resolution, (application to wetting). Manipulation of single molecules: discovery of mechanisms of single molecule water diffusion and cluster formation on metal surfaces, and tip-induced rotation of molecules. Development of novel Photoelectron Spectrometer for studies of surfaces under atmospheric gas pressure conditions, (applications to catalysis and environmental science). Demonstration of the existence and determination of thickness of liquid-like layers on ice below 0C (premelting).

**Program impact:**

Provided insights into origin of frictional energy dissipation in lubricant monolayers and their drainage under pressure (MEMS, Hard Disk lubes). Enabled imaging of liquids with nanometer resolution (previously not possible). Enabled studies of catalysis and environmental science *in situ* using photoelectron spectroscopy. Provide insights into nature of water interaction with metals.

**Interactions:**

Internal: Molecular Environmental Science project at new ALS beam line 11. Surface Science and Catalysis project (Gabor Somorjai). Molecular Foundry initiative (Alivisatos, Frechet, Bokor, Louie, Bertozzi). External: AMES Laboratory: (tribological properties of quasicrystals). Nanoscience Network for Nanoscale Mechanics and Tribology (SNL, UI/MRL, LANL, PNL and ORNL). Univ. Autonoma Madrid, Spain (STM theory). Spanish National Research Council (Thiol monolayers). Univ. Barcelona, Spain: (organic layers). Fritz-Haber-Institut Berlin, Germany: High pressure XPS.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

Plenary lecturer at 18th European Conference on Surface Science (ECOSS-18). Vienna, Austria.

Keynote speaker at the 1<sup>st</sup>. Latin American Symposium on Scanning Probe Microscopy. Sao Carlos, Brazil, 2001.

13 Invited talks since 2001.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

Staff: M. Salmeron (50%), D.F. Ogletree (30%). Postdocs: Toshi Mitsui (100%). Students: M. Rose (100%), Evgueni Fomin (100%).

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$439,000

**FY01 BA** \$463,000

**FY02 BA** \$422,000

**FWP and possible subtask under FWP:** Surface Science Program  
**FWP Number:** KC31

**Program Scope:**

The structure and composition of solid surfaces (metals and polymers) and adsorbed monolayers are determined on the atomic scale with continually increasing spatial and time resolution. Model surfaces are used in these studies, including metal single crystals, and polymer thin films. STM, AFM, and SFG techniques are utilized in most of these studies. The hardness, friction, the mechanism of stretching, and adhesion of polymer surfaces are studied. The rate and selectivity of catalyzed surface reactions are studied using single crystal surfaces, *in situ*, and correlated with surface structure and composition. Instruments have been built that permit molecular level surface studies from high pressures to ultra high vacuum, over fourteen orders of magnitude pressure range using SFG-surface vibrational spectroscopy, STM and AFM. For the first time, the atomic level surface properties can be studied during adsorption and during chemical reactions at high pressures and temperatures and at solid-liquid interfaces.

**Major Program Achievements (over duration of support):**

The high pressure, high temperature scanning tunneling microscope (STM) allowed in-situ examination of surfaces under catalytic conditions in real time and on the molecular scale. Organic molecules on the catalytically active platinum and rhodium surfaces are mobile. When the hydrogenation reaction is poisoned by the co-adsorption of CO the molecular motion is frozen and an ordered adsorbate layer forms surface mobility of molecules and catalytic activity is correlated. SFG studies show that CO dissociation is surface structure sensitive when it occurs on platinum single crystal surfaces. The temperature where CO dissociation occurs coincides with the ignition of CO oxidation. This finding implicates CO dissociation as the primary cause of the ignition of combustion. SFG and AFM studies reveal the molecular mechanism of polymer stretching. Polymers that stretch are two component systems. The hard or crystalline components, which is usually a polymers with high glass transition temperature, act as anchor while the soft polymer component stretch. Thus, the surface composition changes during stretching and the structure of the polymer surface changes as well; it becomes rougher or smoother depending on the relative molecular weights of the hard and soft polymer components. Hydrogels are polymers with high internal water content. Their surface composition changes with humidity as shown by SFG, and their mechanical properties (stiffness, friction coefficient) are also altered with water partial pressure as shown by AFM.

**Program impact:**

Determined the molecular ingredients of surface chemical reactivity; the mobility of surface atoms and molecules, and the metal surface structure. The molecular mechanism of stretching at polymer surfaces was determined. The effects of humidity that modify the surface composition and surface mechanical properties (friction and stiffness) of hydrogels were elucidated.

**Interactions:**

Polymer Technology Group, Berkeley CA; Ocular Sciences, Concord, CA; Basell USA, Inc., Elkton, Chevron Corporation, Richmond, CA. University of California, Berkeley: Prof. Jeff Bokor, Electrical Engineering; Prof. Kyriakos Komvopoulos, Mechanical Engineering; Prof. Song Li and Prof. Tom Buddinger, Bioengineering.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

1998, Wolf Prize in Chemistry, Wolf Foundation  
2002, National Medal of Science  
2002, Named University Professor of all campuses of the University of California  
40 invited talks since January 2001

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

Gabor Somorjai (PI) 10%  
Miguel Salmeron (Sr. Staff Scientist) 20%; Keng-Chang Chou (post-doc) 50%; Joonyeong Kim (post-doc) 100%; Jessica Gaughan; Kevin Hwang; Aric Opdahl; David Tang; and Ji Zhu (students) 50%

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$843,000

**FY01 BA** \$847,000

**FY02 BA** \$772,000

**FWP and possible subtask under FWP:**

Theory for Synchrotron and Other Experiments

**FWP Number:** KC23

**Program Scope:**

This project develops theoretical methods and codes to interpret a variety of data measured at synchrotron facilities, especially the Advanced Light Source, and for experiment more generally. The emphasis is on the experimental techniques of photoelectron diffraction (PD) and x-ray absorption fine structure (XAFS), as well as on ab initio modeling of nanoscale structures and interfaces. Corresponding computer codes are made available to experimentalists. The theoretical/computational work also involves scientists at the National Energy Research Scientific Computing Center (NERSC, now Computational Research Division - CRD) and fits within our global Synchrotron Radiation Research Theory Network.

**Major Program Achievements (over duration of support):**

Structural determination of several important surfaces with photoelectron diffraction and low-energy electron diffraction. Development of new methods and codes for:

- photoelectron diffraction (to generalize and speed up analyses, including of bonding properties in surfaces, and to implement multi-atom resonant photoemission to investigate surface and interface composition);
- holography with electrons (including "differential" holography to significantly improve atomic-scale images) and x-rays (including resonant x-ray fluorescence holography to identify the chemical identity of the atomic neighborhood of fluorescing atoms);
- soft-x-ray standing wave spectroscopy (to probe buried interfaces).

**Program impact:**

This project developed theoretical methods and codes that, when applied to the analysis of experimental data (especially from synchrotron radiation), gave new insights into structural, electronic, and magnetic properties of various surfaces and interfaces.

**Interactions:**

Internal at LBNL: groups at Advanced Light Source, Materials Sciences Division, Chemical Sciences Division, Nat'l Energy Research Supercomputing Center/Computational Research Division.

External: groups at U. California Berkeley, U. California Davis, U Washington Seattle, Oregon State U., Sandia Nat'l Lab - Livermore, Ames Lab, Fritz-Haber-Institut (Germany), Techn. U. Berlin (Germany), U. Frankfurt (Germany), U. Kiel (Germany), U. San Sebastian (Spain), U. Lodz (Poland), U. Tokyo (Japan), U. Hong Kong, Nat'l U. Singapore.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Van Hove (FY00-02): Fellow of American Physical Society and American Vacuum Society; on editorial board of 4 international journals (Progress in Surface Science, Surface Review and Letters, Physics of Low-Dimensional Structures, International Journal of Nanoscience); 17 invited talks; co-organizer of 8 international conferences.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

M. Van Hove (PI, 50%), 2 postdocs with own Fellowships.

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA** \$156,000

**FY01 BA** \$165,000

**FY02 BA** \$149,000

**FWP and possible subtask under FWP:**

Multi-component assembly of high surface-area ordered metal-oxide nanocomposites with enhanced catalytic properties.

**FWP Number:** KC31

**Program Scope:** Developing novel synthetic strategies for shape-controlled growth of Au and Pt nanocrystals, ideally with one type of surface exposed only; Assembly of these shaped Au and Pt nanocrystals within ordered porous oxide (SiO<sub>2</sub>, TiO<sub>2</sub>) matrix; Chemical reaction testing on the ordered metal-oxide nanocomposites to examine the effect of surface type of the nanocrystals, interface and surface area on the catalytic activity and selectivity.

**Major Program Achievements (over duration of support):**

Project initiated in July, 2002 with the arrival of the two postdocs.

Synthetic methodology for oriented silica nanowire and nanotube arrays has been developed. These silica nanostructures possess high surface area and are suitable for serving as supporting matrices for Au and Pt nanoparticles.

Currently exploring the synthetic conditions for shaped Au and Pt nanocrystals growth, mainly using surfactants and polymers as growth regulating agents.

Currently searching for compatibility between sol-gel mesoporous silica chemistry and metal nanocrystal colloidal chemistry in order to develop multi-component assembly chemistry for the ordered metal-oxide nanocomposites through a one-pot process.

**Program Impact:**

Enabling the deterministic assembly of high surface-area metal-oxide nanocomposites with enhanced catalytic activity and selectivity.

**Interactions:**

G. Somorjai (Chemistry): Catalytic reaction studies on the high surface-area ordered metal-oxide nanocomposites.

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

Beckman Fellowship (2002)

Texas Christian University Distinguished Lectureship (2002)

30 Invited talks (year 2002)

**Personnel Commitments for FY2002 to Nearest +/-10%:**

P.D. Yang (PI)

C. Hess (postdoc) 30%

H. Song (postdoc) 100%

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA \$0**

**FY01 BA \$50,000**

**FY02 BA \$100,000**

**Laboratory Name:** Lawrence Berkeley National Laboratory  
**B&R Code:** KC020301

**FWP and possible subtask under FWP:** Interfacing nanostructures: The Design, Synthesis, Characterization, and Application of Functionalized Nanotubes  
**FWP Number:** KC31

**Program Scope:**

*Ab-initio* quantum mechanical calculations to predict new materials structures and relate them to electronic structure and mechanical and thermal properties of interfacing nanostructures. Experimental synthesis of novel hybrid nanomaterials such as coated nanotubes and nanoparticles, internally filled nanotubes and nanostructures, and end- or sidewall-linked nanotubes. Characterization using SEM, TEM, STM, AFM, XRD, mechanical properties, and transport properties. Nanoscale device fabrication and testing using hybrid nanostructures. Strong interdisciplinary interactions between physics, chemistry, and biology.

**Major Program Achievements (over duration of support):**

Prediction of electronic and mechanical properties of hybrid nanostructures including carbon nanotube peapods. Synthesis of carbon peapods and characterization of properties using TEM and transport measurements. Synthesis of BN silo crystal structures.

**Program impact:**

Invention of silo crystal structures (using BN nanotubes filled with fullerene molecules as prototype).

**Interactions:**

Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory

External: University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain

**Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):**

**A. Zettl** – Fellow of APS, Sloan Fellow, Presidential Young Investigator Award, Miller Professor, IBM Faculty Development Award, LBNL Outstanding Performance Award. 20 Invited talks since 2000.

**M. L. Cohen** – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; APS Buckley Prize; DOE Outstanding Accomplishment in Solid State Physics Award; DOE Sustained Outstanding Accomplishment in Solid State Physics Award; APS Lilienfeld Prize; U.S. National Medal of Science; ISI's top 100 most-cited physicists; 25 invited talks since 2000.

**S. G. Louie** – Fellow of APS; Sloan Fellow; Guggenheim Fellow; DOE Sustained Outstanding Research in Solid State Physics Award; APS Aneesur Rahman Prize; APS Davisson-Germer Prize; ISI's top 100 most-cited physicists; 45 invited talks since 2000.

**M. Crommie** – Sloan Fellow, NSF Young Investigator Award. 9 Invited talks since 2000.

**Bertozzi, Bustamante, Clarke** Biological Sciences studies just starting

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

1 Principal Investigator ( <b>Zettl</b> )	10%
6 faculty scientists (Cohen, Louie, Crommie, Clarke, Bustamante, Bertozzi)	10%
3 Post Docs (Aloni 50%, Andrea Trave 100%, Katsumi Nagoaka 50%)	200%
4 grad students: Ryan Yamachika 100%, Xing Chen 100%, C-W. Chang 50%, Mickelson 50%,	300%
1 undergrad student: M. Griffo (50%)	50%

**Authorized Budget (BA) for FY00, FY01, FY02:**

<b>FY00 BA \$</b>	<b>FY01 BA \$700,000</b>	<b>FY02 BA \$640,000</b>
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**FWP and possible subtask under FWP:**  
Novel  $sp^2$ -bonded Materials

**FWP Number:** KC31

**Program Scope:**

Ab-initio quantum mechanical calculations to predict new materials structures and relate them to electronic structure and mechanical and thermal properties. Experimental synthesis of novel  $sp^2$ -bonded materials, and characterization using SEM, TEM, STM, AFM, XRD, mechanical properties, and transport properties. Nanoscale device fabrication and testing. Strong connection between theory and experiment.

**Major Program Achievements (over duration of support):**

Prediction of new nanostructures including  $BxCyNz$ , CN, and GaSe nanotubes and nanoparticles. Theoretical analysis of nanotube devices and crossed tube junctions made and electronic structure of carbon nanotubes and ropes performed. Successful experimental synthesis of BN double-walled nanotubes and nanococoons, nanotube rectifiers, matrix field emission sources, n- and p-type nanotube transistors, and crossed tube devices. Thermopower and thermal conductivity of nanotubes and nonlinear conductance of nanotubes determined. Nanobearings fabricated from nanotubes and frictional properties determined. Young's modulus of carbon and BN nanotubes determined. Electron holography of field-emitting nanotube performed. Oxygen sensitivity of nanotubes discovered. New fullerene-like materials synthesized. STM studies of nanotube junctions and fullerenes performed.

**Program impact:**

First experimental demonstration of nanotube electronic device and nanotube nanobearing. First demonstration of nanotube chemical sensor. Discovery of BN nanotubes and nanoparticles

**Interactions:**

Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory

External: University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, SUNY Stony Brook, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

**A. Zettl** – Fellow of APS, Sloan Fellow, Presidential Young Investigator Award, Miller Professor, IBM Faculty Development Award, LBNL Outstanding Performance Award. 20 Invited talks since 2000.

**M. L. Cohen** – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; APS Buckley Prize; DOE Outstanding Accomplishment in Solid State Physics Award; DOE Sustained Outstanding Accomplishment in Solid State Physics Award; APS Lilienfeld Prize; U.S. National Medal of Science; ISI's top 100 most-cited physicists; 25 invited talks since 2000.

**S. G. Louie** – Fellow of APS; Sloan Fellow; Guggenheim Fellow; DOE Sustained Outstanding Research in Solid State Physics Award; APS Aneesur Rahman Prize; APS Davisson-Germer Prize; ISI's top 100 most-cited physicists; 45 invited talks since 2000.

**R.O. Ritchie** – Fellow, Royal Academy of Engineering, Member, National Academy of Engineering.

**M. Crommie** – Sloan Fellow, NSF Young Investigator Award. 9 Invited talks since 2000.

**Personnel Commitments for FY2002 to Nearest +/- 10%:**

Principal Investigator (Zettl)	25%	1 Undergrad Student (Griffo)	50%
3 Faculty Scientist (Cohen, Louie, Ritchie)	10%		
1 Faculty Scientist (Crommie)	15%		
1 Staff Scientist (Dahmen)	5%		
3 Post Docs (Aloni 50%, Regan 100%, P. Tangney 50%)			
200%			
3 Grad Students (Grobis 100%, Xinghua Lu 100%, Mickelson 50%)			
250%			

**Authorized Budget (BA) for FY00, FY01, FY02:**

**FY00 BA \$689,000**

**FY01 BA \$693,000**

**FY02 BA \$643,000**

**Laboratory Name:** Lawrence Berkeley National Laboratory  
**B&R Code:** KC0203010

**FWP and possible subtask under FWP:** Directed Growth of Ordered Nanostructures (Crystals)

**FWP Number:** KC31

**Program Scope:** Synthesis of nanotube crystals using a variety of CVD, arc-plasma, laser ablation and high pressure, high magnetic field methods with fullerenes as carbon source for carbon nanotubes and boron-compounds for BN nanotube crystals. Detailed TEM analysis including chemical composition, electron and x-ray diffraction studies. Develop reliable model for prediction of and analysis of diffraction patterns.

**Major Program Achievements (over duration of support):** IBM results reproduced (but interpreted not as carbon nanotube crystals, but rather as other compound nanocrystals). Detailed diffraction pattern predictions made and compared to published and new diffraction results. New methods for "solid state" synthesis of nanotubes successfully demonstrated.

**Program Impact:** IBM results shown to be incorrect, but foundation set for synthesis of such nanotube crystals with proper diffraction interpretation checks in place. New solid state synthesis methods demonstrated for nanoparticle growth.

**Interactions:** Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory  
External: University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, (Geohagen) Oakridge National Laboratory, (Smalley) Rice University, (Gimzewski) UCLA

**Recognitions, Honors and Awards (at least in some part attributable to support under this program):**

**A. Zettl** – Fellow of APS, Sloan Fellow, Presidential Young Investigator Award, Miller Professor, IBM Faculty Development Award, LBNL Outstanding Performance Award. 20 Invited talks since 2000.

**Personnel Commitments for FY2002 to Nearest +/-10%: (?)**

1 Principal Investigator ( <b>Zettl</b> )	40%
2 PostDoc (Aloni 50%, AN Other 50%)	100%
4 Graduate Students: Fennimore 100%, Yuzvinsky 100%, Chang 50%, Ishigami 50%	300%

**Authorized Budget (BA) for FY00, FY01, FY02:**

FY00 BA \$	FY01 BA \$200,000	FY02 BA \$400,000
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